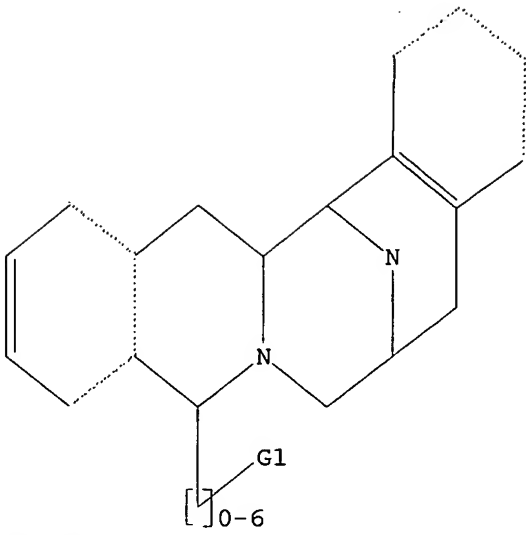
R



G1 O,S

Structure attributes must be viewed using STN Express query preparation.

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=> s l4
SAMPLE SEARCH INITIATED 19:07:38 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     38 TO ITERATE

100.0% PROCESSED      38 ITERATIONS                                4 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          391 TO     1129
PROJECTED ANSWERS:               4 TO      200

L5             4 SEA SSS SAM L4

=> s l4 sss full
FULL SEARCH INITIATED 19:07:47 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    695 TO ITERATE

100.0% PROCESSED     695 ITERATIONS                               92 ANSWERS
SEARCH TIME: 00.00.01

L6            92 SEA SSS FUL L4

=> file caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               323.09     323.30

FILE 'CAPLUS' ENTERED AT 19:07:54 ON 15 FEB 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 15 Feb 2005 VOL 142 ISS 8
FILE LAST UPDATED: 14 Feb 2005 (20050214/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

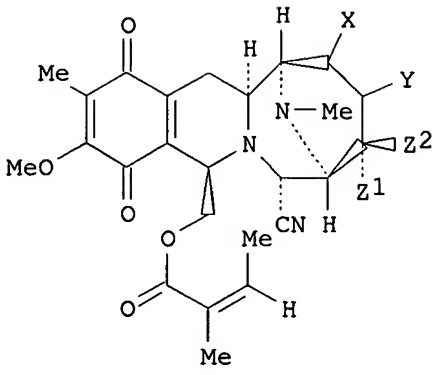
=> s l6
L7 26 L6

=> d l7 1-26 ibib abs hitstr

L7 ANSWER 1 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:680266 CAPLUS
DOCUMENT NUMBER: 141:167764
TITLE: Renieramycins, their isolation from Xestospongia species, and anticancer agents containing them
INVENTOR(S): Kubo, Yotoku; Saito, Naoki; Pummangura, Sunibhond; Suwanborirux, Khanit
PATENT ASSIGNEE(S): Chulalongkorn University, Japan; National Center for Genetic Engineering and Biotechnology; National Science and Technology Development Agency
SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004231552	A2	20040819	JP 2003-20821	20030129
PRIORITY APPLN. INFO.:			JP 2003-20821	20030129

OTHER SOURCE(S): MARPAT 141:167764
GI



I

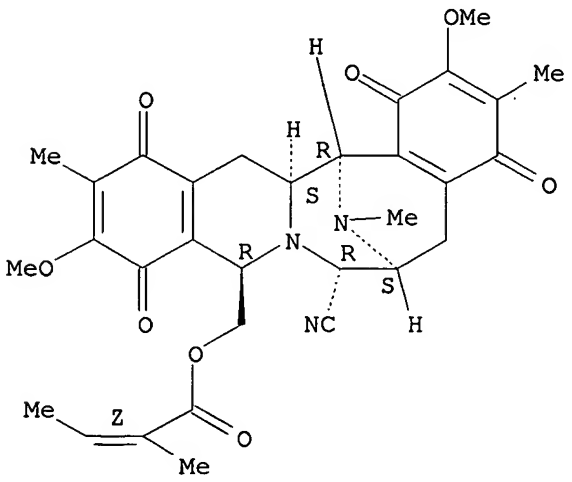
AB Renieramycins I [XY = COC(OMe):CMeCO, C(OH):C(OMe)CMe:C(OH); Z1, Z2 = H, OH, C1-6 alkoxy, acetoxyl; Z1Z2 = O] are isolated from blue sponge of Xestospongia sp. via homogenization, treatment with KCN while adjusting pH to 5.5-7.5 using phosphate buffers, extraction with MeOH, and purification by chromatog. Renieramycin M [I; XY = COC(OMe):CMeCO, Z1 = Z2 = H] in vitro inhibited human pulmonary cancer cells QG 56 with IC50 of 1.9, vs. 5.5, for saframycin A.

IT **631913-64-9P**, Renieramycin M **631913-65-0P**, Renieramycin N
RL: PAC (Pharmacological activity); PUR (Purification or recovery); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(anticancer agents containing renieramycins from Xestospongia sp.)

RN 631913-64-9 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(6S,7R,9R,14aS,15R)-7-cyano-1,5,6,7,9,10,13,14,14a,15-decahydro-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.

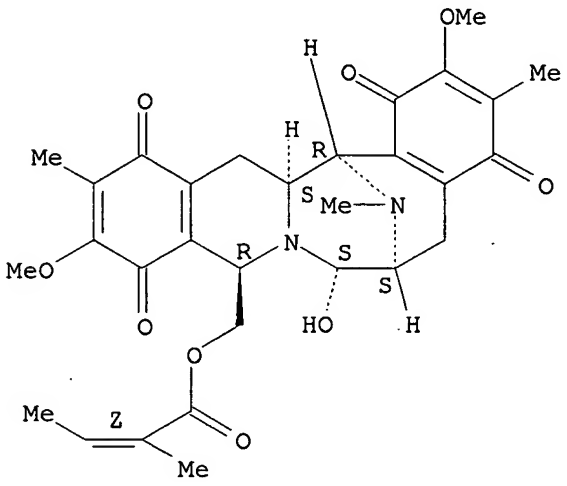


RN 631913-65-0 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(5S,6R,7R,9R,14aS,15R)-7-cyano-6,7,9,10,13,14,14a,15-octahydro-1,4,5-trihydroxy-2,11-dimethoxy-3,12,16-

(anticancer agents containing renieramycins from Xestospongia sp.)
RN 123641-95-2 CAPLUS
CN 2-Butenoic acid, 2-methyl-, [(6S,7S,9R,14aS,15R)-1,5,6,7,9,10,13,14,14a,15-decahydro-7-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



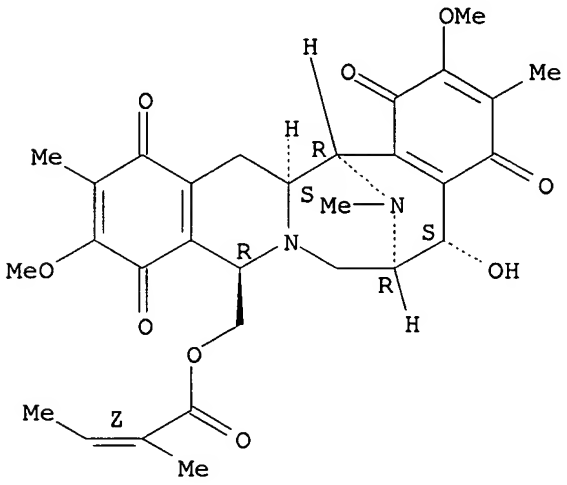
L7 ANSWER 2 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:595237 CAPLUS
DOCUMENT NUMBER: 142:32489
TITLE: identification of renieramycin A as an antileishmanial substance in a marine sponge Neopetrosia sp
AUTHOR(S): Nakao, Yoichi; Shiroiwa, Takeru; Murayama, Shuhei; Matsunaga, Shigeki; Goto, Yasuyuki; Matsumoto, Yoshitsugu; Fusetani, Nobuhiro
CORPORATE SOURCE: Lab. Aquatic Natural Products Chem., Grad. Sch. Agricultural and Life Sci., The Univ. Tokyo, Tokyo, 113-8657, Japan
SOURCE: Marine Drugs (2004), 2(2), 55-62
CODEN: MDARE6; ISSN: 1660-3397
URL: http://www.mdpi.net/marinedrugs/papers/papers04/md202055.pdf
PUBLISHER: MDPI Center
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English
AB The newly developed assay system using recombinant Leishrnania amazonensis expressing enhanced green fluorescent protein (La/egfr) has been applied to the screening of Japanese marine sponges for antileishmanial activity. Bioassay-guided fractionation of an active sponge Neopetrosia sp. afforded an active compound which was identified as renieramycin A by spectroscopic anal. It inhibited La/egf with an IC50 value of 0.2 μg/mL.
IT **79664-60-1P**, Renieramycin A
RL: NPO (Natural product occurrence); PAC (Pharmacological activity); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); USES (Uses)
(renieramycin A showed dose-dependent inhibition against Leishmania amazonensis expressing enhanced green fluorescent protein in new assay,

indicating antileishmanial activity and also showed cytotoxicity against P388 murine leukemia cell)

RN 79664-60-1 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(5S,6R,9R,14aS,15R)-1,5,6,7,9,10,13,14,14a,15-decahydro-5-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:465167 CAPLUS

DOCUMENT NUMBER: 141:120456

TITLE: Chemistry of renieramycins. Part 5. Structure elucidation of renieramycin-type derivatives O, Q, R, and S from Thai marine sponge Xestospongia species pretreated with potassium cyanide

AUTHOR(S): Amnuoypol, Surattana; Suwanborirux, Khanit; Pummangura, Sunibhond; Kubo, Akinori; Tanaka, Chieko; Saito, Naoki

CORPORATE SOURCE: Bioactive Marine Natural Products Chemistry Research Unit (BMNCU), Department of Pharmacognosy, Faculty of Pharmaceutical Sciences, Chulalongkorn University, Bangkok, 10330, Thailand

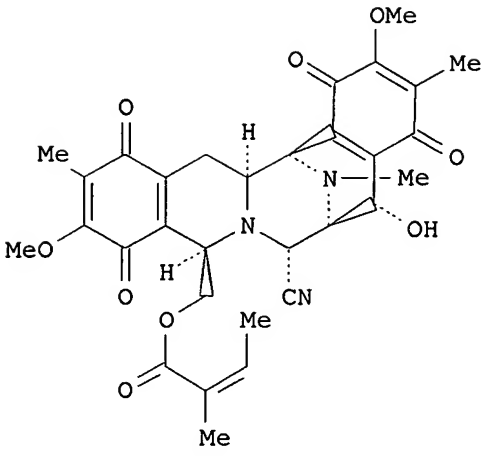
SOURCE: Journal of Natural Products (2004), 67(6), 1023-1028
CODEN: JNPRDF; ISSN: 0163-3864

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

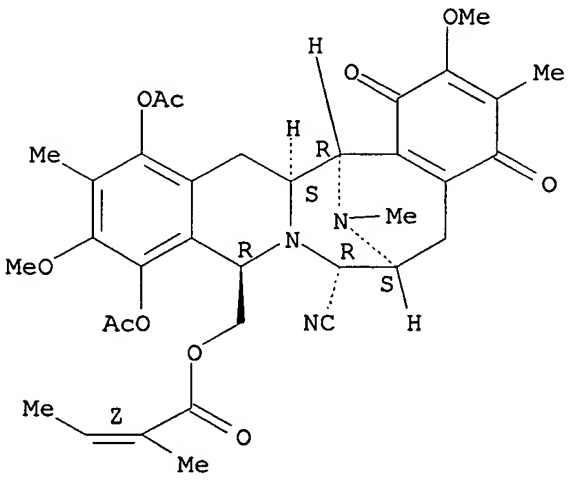
AB Four minor renieramycin-type derivs., including renieramycins O (I) and Q-S, were isolated from the sponge Xestospongia sp. pretreated with potassium cyanide. Their structures were elucidated by comparison of spectral data with those of recently reported renieramycins M and N. The results of transformation and cytotoxicity measurements are also described.

IT **723308-87-0P**
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(antitumor activity of)

RN 723308-87-0 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(6S,7R,9R,14aS,15R)-10,13-bis(acetyloxy)-7-cyano-1,5,6,7,9,14,14a,15-octahydro-2,11-dimethoxy-3,12,16-trimethyl-1,4-dioxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)-(9CI) (CA INDEX NAME)

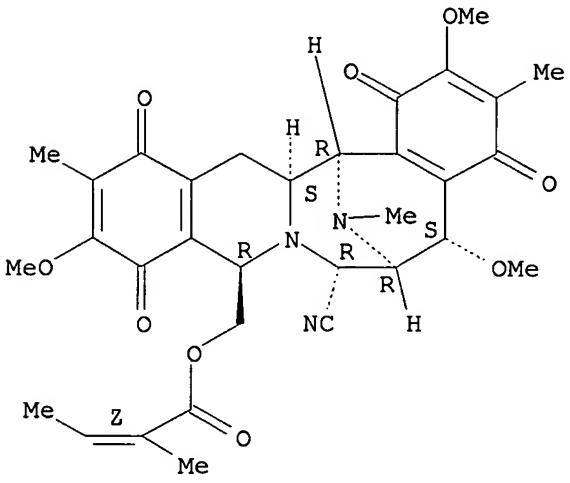
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



IT **631913-65-0**, Renieramycin N
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);

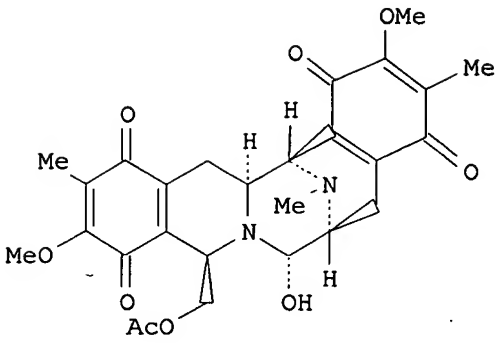
RN 724707-54-4 CAPLUS
CN 2-Butenoic acid, 2-methyl-, [(5S,6R,7R,9R,14aS,15R)-7-cyano-1,5,6,7,9,10,13,14,14a,15-decahydro-2,5,11-trimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:278842 CAPLUS
DOCUMENT NUMBER: 141:38759
TITLE: Chemistry of renieramycins. Part 6: Transformation of renieramycin M into jorumycin and renieramycin J including oxidative degradation products, mimosamycin, renierone, and renierol acetate
AUTHOR(S): Saito, Naoki; Tanaka, Chieko; Koizumi, Yu-ichi; Suwanborirux, Khanit; Amnuoypol, Surattana; Pummangura, Sunibhond; Kubo, Akinori
CORPORATE SOURCE: Meiji Pharmaceutical University, Kiyose, Tokyo, 204-8588, Japan
SOURCE: Tetrahedron (2004), 60(17), 3873-3881
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:38759
GI



I

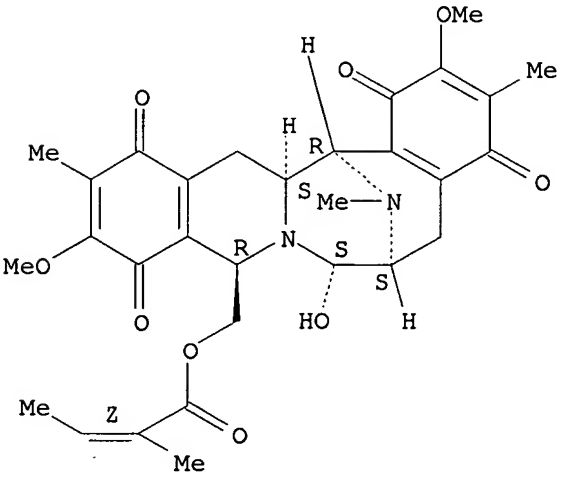
AB The transformation of renieramycin M into renieramycin J and jorumycin (I) is presented along with the results of antiproliferative assay data. The chemical stability and the oxidative degradation of I and renieramycin E to generate simple isoquinoline alkaloids, such as mimosamycin, renierol acetate, and renierone are also described. The cytotoxicity IC50 of jorumycin and derivs. was determined

IT **123641-95-2**, Renieramycin e **631913-64-9**, Renieramycin M
RL: PAC (Pharmacological activity); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(transformation of renieramycin M into jorumycin and renieramycin J including oxidative degradation products, mimosamycin, renierone, and renierol acetate)

RN 123641-95-2 CAPLUS

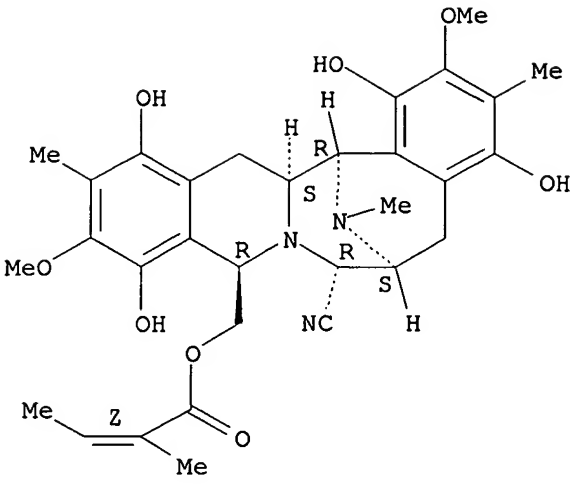
CN 2-Butenoic acid, 2-methyl-, [(6S,7S,9R,14aS,15R)-1,5,6,7,9,10,13,14,14a,15-decahydro-7-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 631913-64-9 CAPLUS

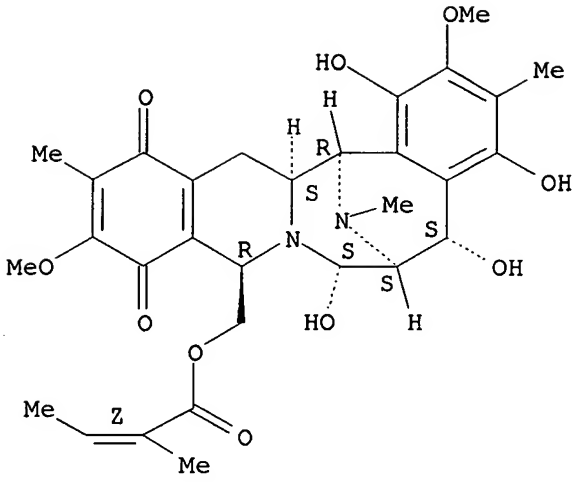
CN 2-Butenoic acid, 2-methyl-, [(6S,7R,9R,14aS,15R)-7-cyano-1,5,6,7,9,10,13,14,14a,15-decahydro-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

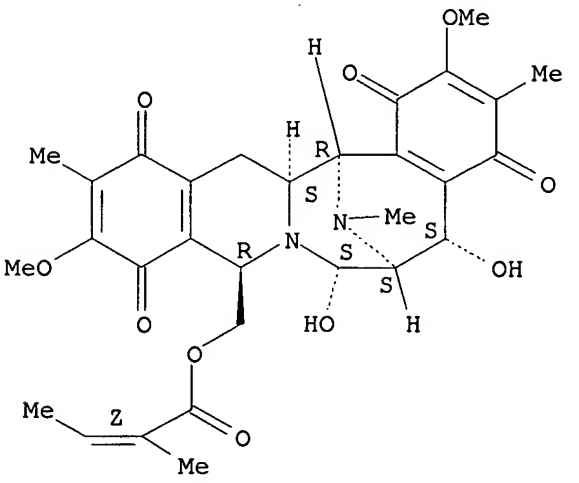
L7 ANSWER 5 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:133034 CAPLUS
DOCUMENT NUMBER: 141:292493
TITLE: Renieramycin P, a highly cytotoxic tetrahydroisoquinoline alkaloid, from a marine sponge Neopetrosia sp. [Erratum to document cited in CA139:227487]
AUTHOR(S): Oku, Naoya; Matsunaga, Shigeki; van Soest, Rob W. M.; Fusetani, Nobuhiro
CORPORATE SOURCE: Laboratory of Aquatic Natural Products Chemistry, Graduate School of Agricultural and Life Sciences, The University of Tokyo, Bunkyo, Tokyo, 113-8657, Japan
SOURCE: Journal of Natural Products (2004), 67(3), 526
CODEN: JNPRDF; ISSN: 0163-3864
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The term "renieramycin J" should read as "renieramycin P" throughout the paper.
IT **593280-18-3P**
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PAC (Pharmacological activity); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(cytotoxic tetrahydroisoquinoline alkaloid from marine sponge Neopetrosia sp. (Erratum))
RN 593280-18-3 CAPLUS
CN 2-Butenoic acid, 2-methyl-, [(5S,6S,7S,9R,14aS,15R)-6,7,9,10,13,14,14a,15-octahydro-1,4,5,7-tetrahydroxy-2,11-dimethoxy-3,12,16-trimethyl-10,13-dioxo-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



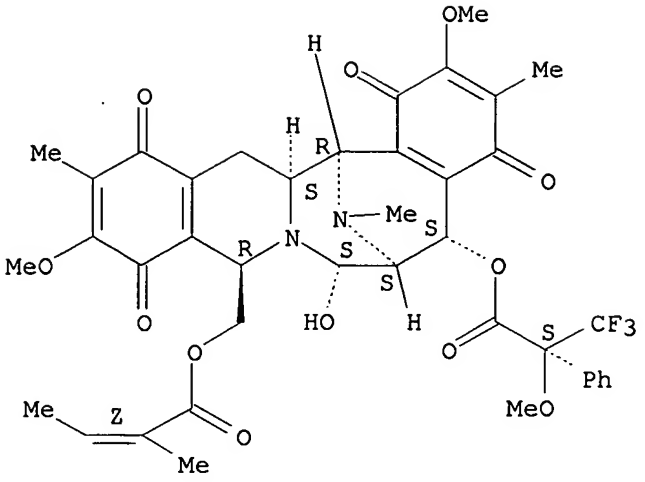
IT **592532-76-8P 592532-77-9P 592532-78-0P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and properties of (Erratum))
RN 592532-76-8 CAPLUS
CN 2-Butenoic acid, 2-methyl-, [(5S,6S,7S,9R,14aS,15R)-
1,5,6,7,9,10,13,14,14a,15-decahydro-5,7-dihydroxy-2,11-dimethoxy-3,12,16-
trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-
yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



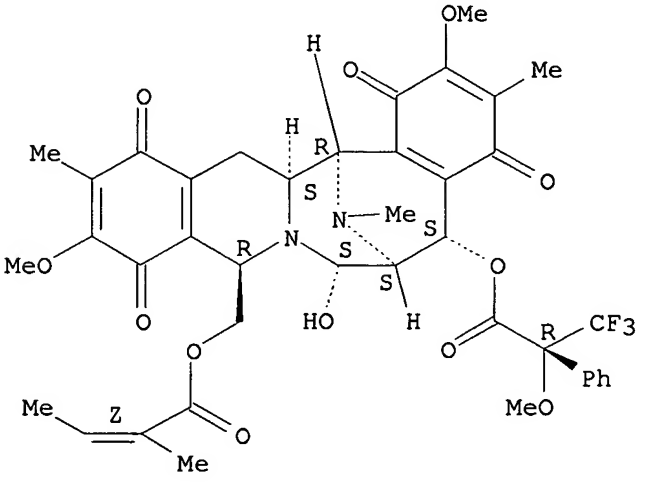
RN 592532-77-9 CAPLUS
CN Benzeneacetic acid, α-methoxy-α-(trifluoromethyl)-,
(5S,6S,7S,9R,14aS,15R)-1,5,6,7,9,10,13,14,14a,15-decahydro-7-hydroxy-2,11-
dimethoxy-3,12,16-trimethyl-9-[[[(2Z)-2-methyl-1-oxo-2-butenyl]oxy]methyl]-
1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-5-yl ester,
(αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 592532-78-0 CAPLUS
CN Benzeneacetic acid, α-methoxy-α-(trifluoromethyl)-, (5S,6S,7S,9R,14aS,15R)-1,5,6,7,9,10,13,14,14a,15-decahydro-7-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-9-[[[(2Z)-2-methyl-1-oxo-2-butenyl]oxy]methyl]-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-5-yl ester, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L7 ANSWER 6 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:832855 CAPLUS
DOCUMENT NUMBER: 140:14944
TITLE: Chemistry of renieramycins. Part 3. Isolation and structure of stabilized renieramycin type derivatives possessing antitumor activity from Thai sponge Xestospongia species, pretreated with potassium cyanide
AUTHOR(S): Suwanborirux, Khanit; Amnuoypol, Surattana; Plubrukarn, Anuchit; Pummangura, Sunibhond; Kubo, Akinori; Tanaka, Chieko; Saito, Naoki

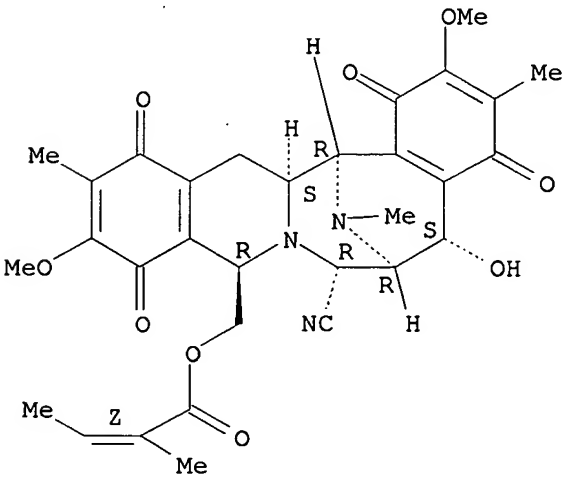
CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Chulalongkorn University, Bangkok, 10330, Thailand
SOURCE: Journal of Natural Products (2003), 66(11), 1441-1446
CODEN: JNPRDF; ISSN: 0163-3864
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

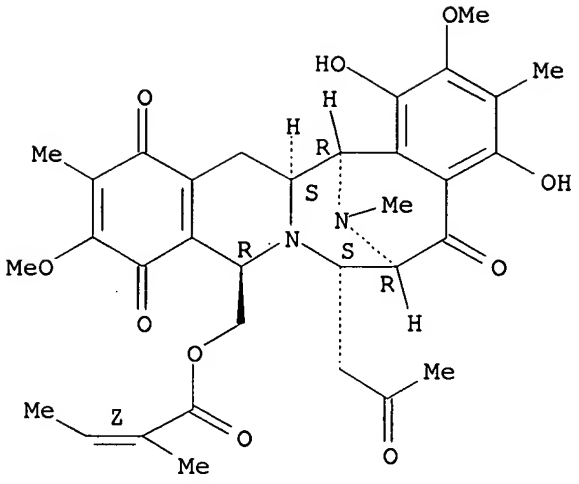
AB Renieramycins M (I) and N (II) were isolated from the Thai sponge Xestospongia sp., pretreated with potassium cyanide in methanolic buffer solution, and their structures and relative stereochemistries were elucidated on the basis of spectroscopic data. This strategy is the first example of the gram-scale preparation of this series of compds. and presents a potential solution for increasing the gram-scale supply of novel natural products from marine sources.

IT **631913-68-3P**, Renieramycin O
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(oxidation product of renieramycin N)
RN 631913-68-3 CAPLUS
CN 2-Butenoic acid, 2-methyl-, [(5S,6R,7R,9R,14aS,15R)-7-cyano-1,5,6,7,9,10,13,14,14a,15-decahydro-5-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.

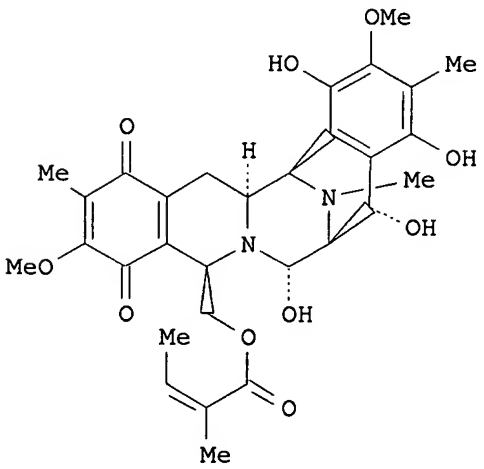


IT **123641-95-2P**, Renieramycin E
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(renieramycin M transformation product)
RN 123641-95-2 CAPLUS
CN 2-Butenoic acid, 2-methyl-, [(6S,7S,9R,14aS,15R)-1,5,6,7,9,10,13,14,14a,15-decahydro-7-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 7 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:585736 CAPLUS
DOCUMENT NUMBER: 139:227487
TITLE: Renieramycin J, a highly cytotoxic tetrahydroisoquinoline alkaloid, from a marine sponge Neopetrosia sp.
AUTHOR(S): Oku, Naoya; Matsunaga, Shigeki; Van Soest, Rob W. M.; Fusetani, Nobuhiro
CORPORATE SOURCE: Laboratory of Aquatic Natural Products Chemistry, Graduate School of Agricultural and Life Sciences, The University of Tokyo, Bunkyo, Tokyo, 113-8657, Japan
SOURCE: Journal of Natural Products (2003), 66(8), 1136-1139
CODEN: JNPRDF; ISSN: 0163-3864
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

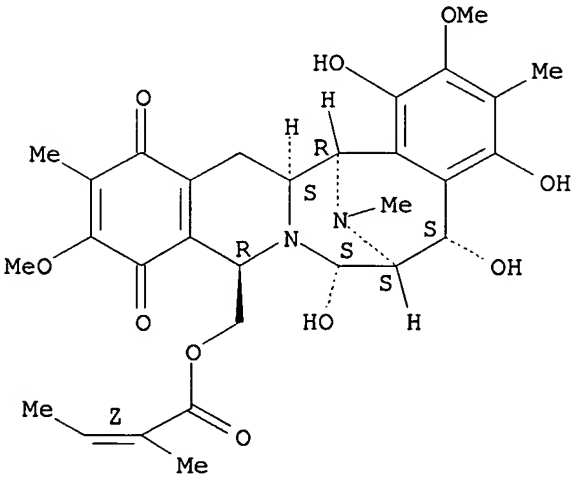
AB Renieramycin J (I), a new tetrahydroisoquinoline alkaloid, has been isolated from a marine sponge Neopetrosia sp. as a potent cytotoxin that induced morphol. changes in 3Y1 cells. Such changes are characteristic of RNA and/or protein synthesis inhibitors. The structure of I including the absolute stereochem. was determined by spectroscopic and chemical methods.

IT **593280-18-3P**, Renieramycin J (Neopetrosia)
RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PAC (Pharmacological activity); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(cytotoxic tetrahydroisoquinoline alkaloid from marine sponge Neopetrosia sp.)

RN 593280-18-3 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(5S,6S,7S,9R,14aS,15R)-6,7,9,10,13,14,14a,15-octahydro-1,4,5,7-tetrahydroxy-2,11-dimethoxy-3,12,16-trimethyl-10,13-dioxo-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.

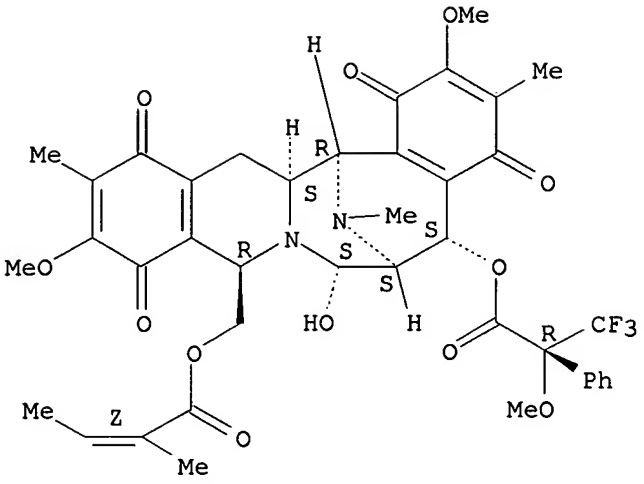


IT **592532-76-8P 592532-77-9P 592532-78-0P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and properties of)

RN 592532-76-8 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(5S,6S,7S,9R,14aS,15R)-1,5,6,7,9,10,13,14,14a,15-decahydro-5,7-dihydroxy-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 8 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:955154 CAPLUS

DOCUMENT NUMBER: 138:205241

TITLE: Chemistry of renieramycins. Part 2. Partial reduction and nucleophilic substitution of hexahydro-1,5-imino-4-oxo-3-benzazocine-7,10-dione: Promising method to construct renieramycin J from renieramycin G via renieramycin E

AUTHOR(S): Koizumi, Yu-ichi; Kubo, Akinori; Suwanborirux, Khanit; Saito, Naoki

CORPORATE SOURCE: Meiji Pharmaceutical University, Tokyo, 204-8588, Japan

SOURCE: Heterocycles (2002), 57(12), 2345-2355
CODEN: HTCYAM; ISSN: 0385-5414

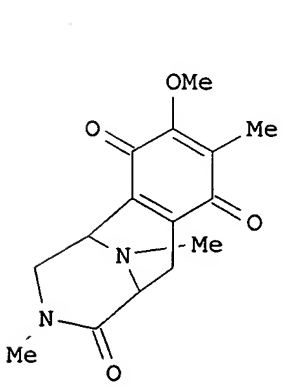
PUBLISHER: Japan Institute of Heterocyclic Chemistry

DOCUMENT TYPE: Journal

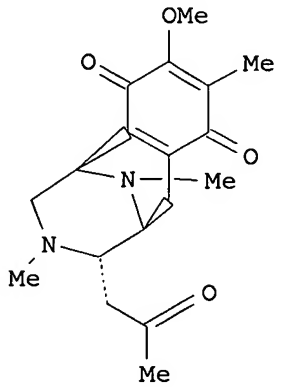
LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:205241

GI



I



II

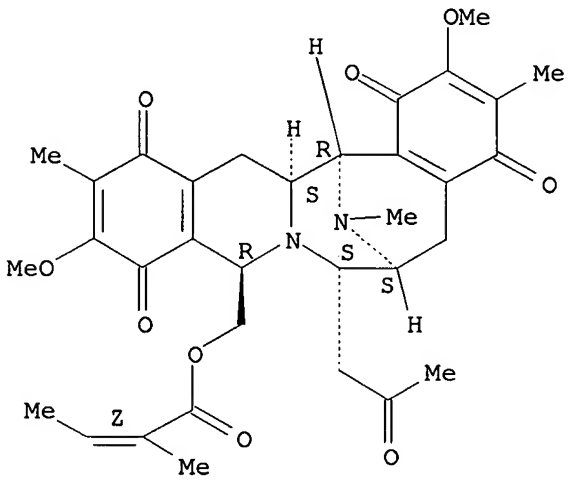
AB The conversion of 1,2,3,4,5,6,7,10-octahydro-9-methoxy-3,8,11-trimethyl-1,5-imino-3- benzazocine-4,7,10-trione (I) to the corresponding alkylated compound at C-21 position, II, as an ABC ring model of renieramycin J is described. This is a promising method for converting renieramycin G into renieramycin J via renieramycin E. The antitumor activity of some of the prepared compds. was evaluated in several cancer cell lines.

IT **500111-59-1P**, Renieramycin J
RL: PNU (Preparation, unclassified); PREP (Preparation)
(preparation of an ABC ring model of renieramycin J from a lactam carbonyl via partial reduction and nucleophilic substitution)

RN 500111-59-1 CAPLUS

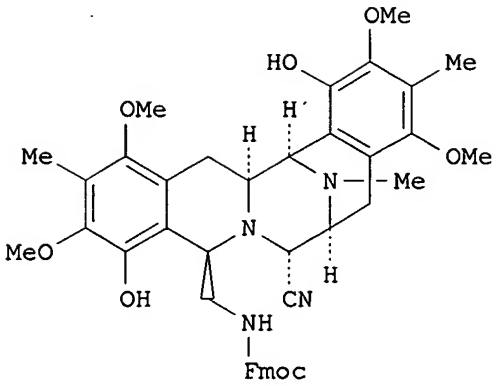
CN 2-Butenoic acid, 2-methyl-, [(6S,7S,9R,14aS,15R)-1,5,6,7,9,10,13,14,14a,15-decahydro-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-7-(2-oxopropyl)-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 9 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:765217 CAPLUS
DOCUMENT NUMBER: 138:14135
TITLE: A Solid-Supported, Enantioselective Synthesis Suitable for the Rapid Preparation of Large Numbers of Diverse Structural Analogues of (-)-Saframycin A
AUTHOR(S): Myers, Andrew G.; Lanman, Brian A.
CORPORATE SOURCE: Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, 02138, USA
SOURCE: Journal of the American Chemical Society (2002), 124(44), 12969-12971
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:14135
GI



I

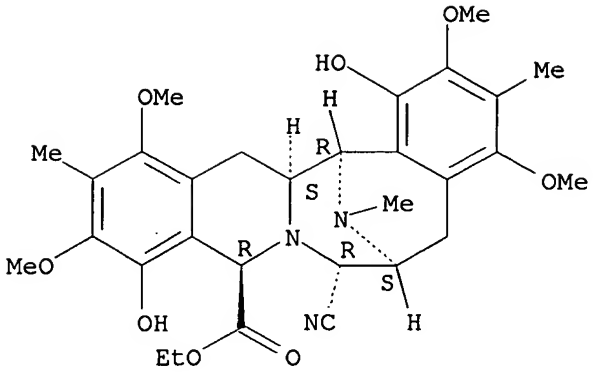
AB A 10-step solid-supported, enantioselective synthesis suitable for the rapid preparation of large nos. of diverse structural analogs of saframycin A is described. The synthetic route, which bears analogy to solid-phase peptide synthesis, involves the directed condensation of N-protected α-amino aldehyde reactants, e.g. N-Fmoc-glycinal (Fmoc = 9-fluorenylmethoxycarbonyl). A novel dual linker, (S)-2-[4-(tert-butyldimethylsilyloxy)-1-butyl]morpholine, was developed for attachment of intermediates to the solid support via a C-protective group, a substituted morpholino nitrile derivative The route employs a novel diastereospecific cyclorelease mechanism, supports structural variation at multiple sites in the saframycin core, and obviates the need for chromatog. purification of the products or any intermediate. To demonstrate the feasibility of structural variation at multiple sites, a matrix of 16 saframycin A analogs, e.g. I, was prepared by parallel synthesis with simultaneous variation of two sites. This work is notable not only as a preliminary step toward large-scale library construction but also as an example of the use of sequential stereoselective C-C bond-forming reactions on the solid phase for the preparation of natural product analogs.

IT **429687-39-8P 477566-41-9P 477566-42-0P 477566-43-1P 477566-44-2P 477566-56-6P 477566-57-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. synthesis of (-)-saframycin A analogs via solid-supported combinatorial chemical using a directed condensation of N-protected amino aldehydes with (silyloxybutyl)morpholine dual linker and Pictet-Spengler cyclization)

RN 429687-39-8 CAPLUS

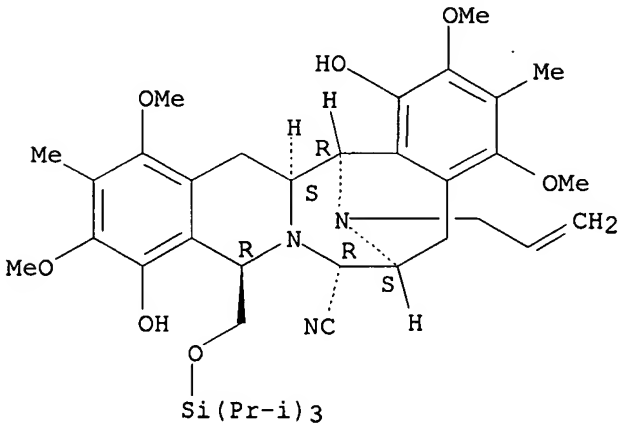
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid, 7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-, ethyl ester, (6S,7R,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



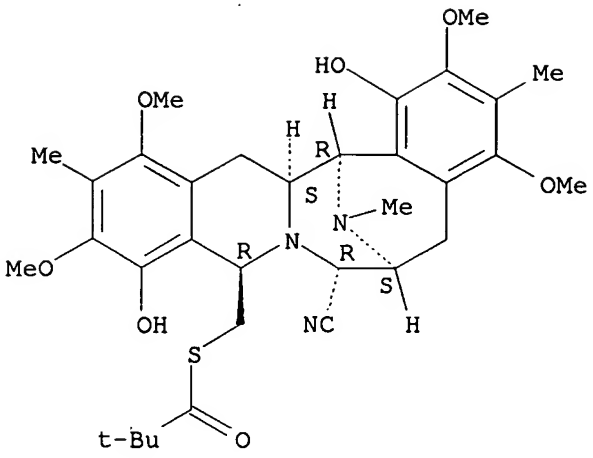
RN 477566-41-9 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7-carbonitrile, 6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12-dimethyl-16-(2-propenyl)-9-[[[tris(1-methylethyl)silyl]oxy]methyl]-, (6S,7R,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 477566-42-0 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7-carbonitrile, 6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12-dimethyl-16-(2-propynyl)-9-[[[tris(1-methylethyl)silyl]oxy]methyl]-, (6S,7R,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



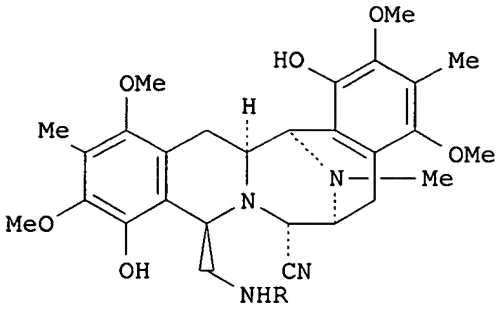
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 10 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:391711 CAPLUS
DOCUMENT NUMBER: 136:401914
TITLE: Preparation of saframycin analogs for pharmaceutical use in the treatment of cancer
INVENTOR(S): Myers, Andrew; Plowright, Alleyn T.; Kung, Daniel W.; Lanman, Brian; Barbay, Joseph; Xing, Chengguo
PATENT ASSIGNEE(S): President and Fellows of Harvard College, USA
SOURCE: PCT Int. Appl., 203 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

Parent

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002040477	A2	20020523	WO 2001-US47399	20011105
WO 2002040477	A3	20030227		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002039565	A5	20020527	AU 2002-39565	20011105
US 2003008873	A1	20030109	US 2001-11466	20011105
US 6809099	B2	20041026		
EP 1339713	A2	20030903	EP 2001-987338	20011105
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004529074	T2	20040924	JP 2002-543487	20011105
US 2004204419	A1	20041014	US 2004-826859	20040416
PRIORITY APPLN. INFO.:			US 2000-245888P	P 20001103
			US 2001-11466	A3 20011105
			WO 2001-US47399	W 20011105

OTHER SOURCE(S): MARPAT 136:401914
GI



I

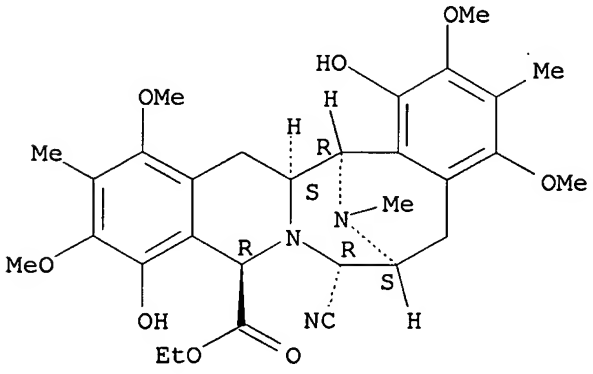
AB Saframycin analogs, such as I [R = H, alkyl, acyl, arylacyl, heteroarylacyl, carboxy, arylsulfonyl, etc.], were prepared for therapeutic use as antitumor agents. Thus, I (R = 2-furanylmethyl) was prepared in 95% yield via condensation of 2-furancarboxaldehyde with the corresponding amine I (R = NH2) using sodium triacetoxyborohydride in MeCN. The amine I (R = H) was prepared via a stereoselective sequence of solid phase synthetic steps. The prepared saframycin analogs were assayed for cancer cell growth inhibition of A375 malignant melanoma and A-459 lung carcinoma cell lines.

IT **429687-39-8P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of saframycin analogs for pharmaceutical use in the treatment of cancer)

RN 429687-39-8 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid, 7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-, ethyl ester, (6S,7R,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 11 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:545697 CAPLUS
DOCUMENT NUMBER: 135:137633
TITLE: Preparation of saframycin-ecteinascidin analogs and

their therapeutic applications

INVENTOR(S): Danishefsky, Samuel J.; Zhou, Bishan

PATENT ASSIGNEE(S): The Trustees of Columbia University in the City of New York, USA

SOURCE: PCT Int. Appl., 115 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

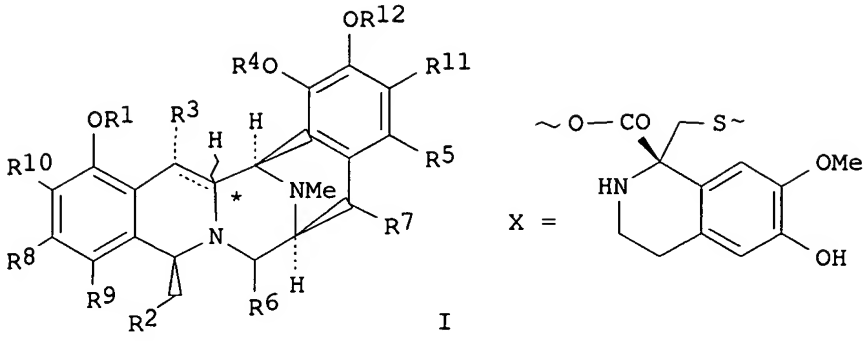
FAMILY ACC. NUM. COUNT: 1

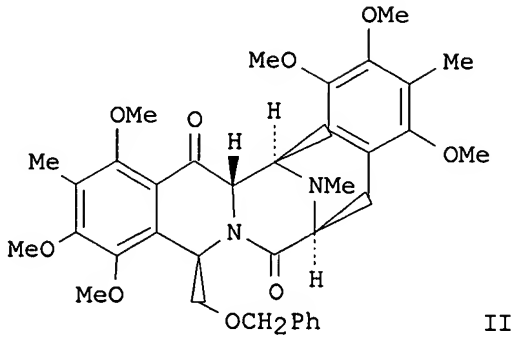
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001053299	A1	20010726	WO 2001-US1877	20010119
WO 2001053299	C2	20021024		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2397597	AA	20010726	CA 2001-2397597	20010119
US 2002025962	A1	20020228	US 2001-765515	20010119
US 6686470	B2	20040203		
EP 1254140	A1	20021106	EP 2001-903151	20010119
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003520801	T2	20030708	JP 2001-553773	20010119
US 2004127709	A1	20040701	US 2003-728580	20031205
PRIORITY APPLN. INFO.:			US 2000-177071P	P 20000119
			US 2001-765515	A3 20010119
			WO 2001-US1877	W 20010119

OTHER SOURCE(S): MARPAT 135:137633

GI





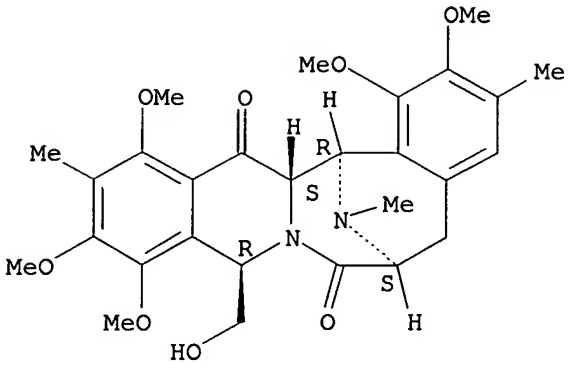
AB Compds. of the saframycin-ecteinascidin series such as I [R1,R4 = H, alkyl, acyl; R3 = =O, OH, ether, sulfide, acyl group such as OC(O)Me, OC(O)Bn and OC(O)Et; R5 = H, halogen, OH, ether, acyl, amide; R6 = =O, OH, OMe, CN, acyloxy; R7 = =O, OH, halogen, ether, acyl; R8 and R9 independently = H, Me, OMe, OEt, CF3, Br, F; R8R9 = OCH2O, five or six membered ring; R10,R11 = Me, OMe, OEt, SMe, SEt; R12 = H, alkyl, acyl; chiral center marked * has the R or the S configuration], were prepared for use as antitumor and antimicrobial agents. Thus, saframycin analog II was prepared via a multistep synthetic sequence starting from 2,4-Dimethoxy-3-methylbenzaldehyde, bromoacetal, 2-hydroxy-4-methoxy-3-methylbenzaldehyde and [[(2E)-4-bromo-2-butenyl]oxy](1,1-dimethylethyl)dimethylsilane. Ecteinascidin 743 I (R1 = Ac, R2R3 = X, R4 = R5 = R7 = H, R6 = α-OH, R8R9 = OCH2O, R10-R12 = Me) was tested for cytotoxicity and antimicrobial activity.

IT **351378-59-1P 351378-84-2P 351378-93-3P**
RL: PNU (Preparation, unclassified); PREP (Preparation)
(attempted synthesis of)

RN 351378-59-1 CAPLUS

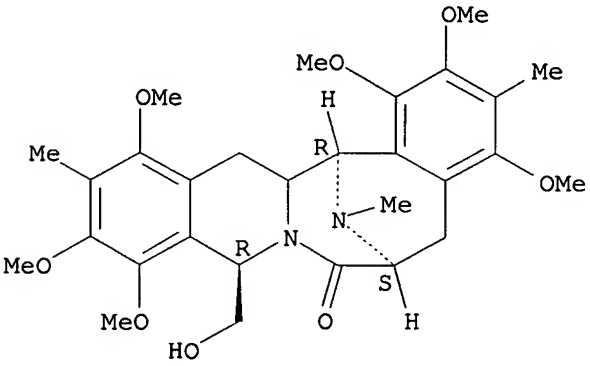
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 14a,15-dihydro-9-(hydroxymethyl)-1,2,10,11,13-pentamethoxy-3,12,16-trimethyl-, (6S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



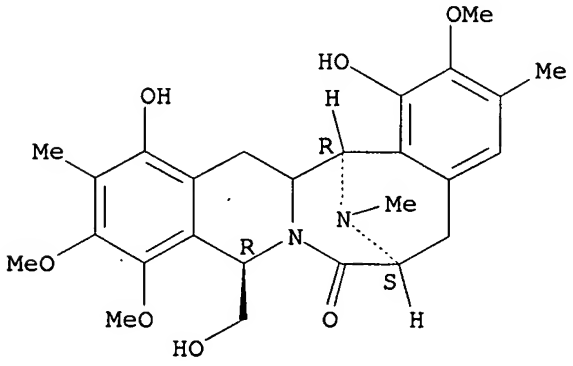
RN 351378-84-2 CAPLUS
CN 6,15-Imino-7H-isoquino[3,2-b][3]benzazocin-7-one, 5,6,9,14,14a,15-hexahydro-9-(hydroxymethyl)-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6S,9R,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 351378-93-3 CAPLUS
CN 6,15-Imino-7H-isoquino[3,2-b][3]benzazocin-7-one, 5,6,9,14,14a,15-hexahydro-1,13-dihydroxy-9-(hydroxymethyl)-2,10,11-trimethoxy-3,12,16-trimethyl-, (6S,9R,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

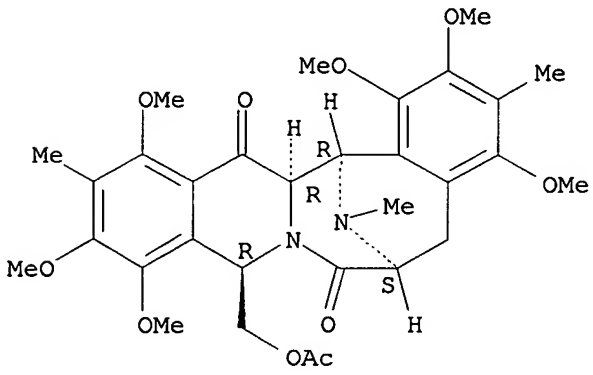


IT **351377-83-8P 351377-84-9P 351377-85-0P**

351377-86-1P 351377-88-3P 351378-45-5P
351379-85-6P 351379-86-7P 351379-88-9P
351379-89-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of saframycin-ecteinascidin analogs and their therapeutic applications)

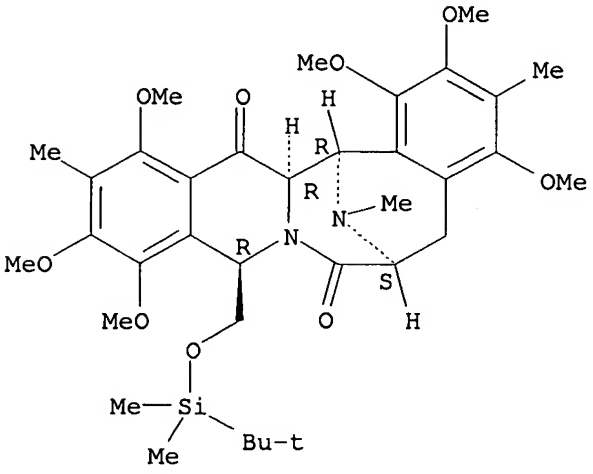
RN 351377-83-8 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 9-[(acetyloxy)methyl]-14a,15-dihydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6S,9R,14aR,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 351377-84-9 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 9-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-14a,15-dihydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6S,9R,14aR,15R)- (9CI) (CA INDEX NAME)

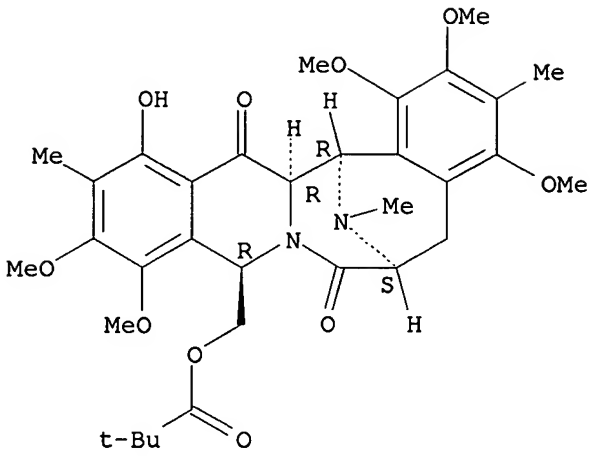
Absolute stereochemistry.



RN 351377-85-0 CAPLUS
CN Propanoic acid, 2,2-dimethyl-, [(6S,9R,14aR,15R)-6,7,9,14,14a,15-hexahydro-13-hydroxy-1,2,4,10,11-pentamethoxy-3,12,16-trimethyl-7,14-dioxo-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester (9CI) (CA INDEX

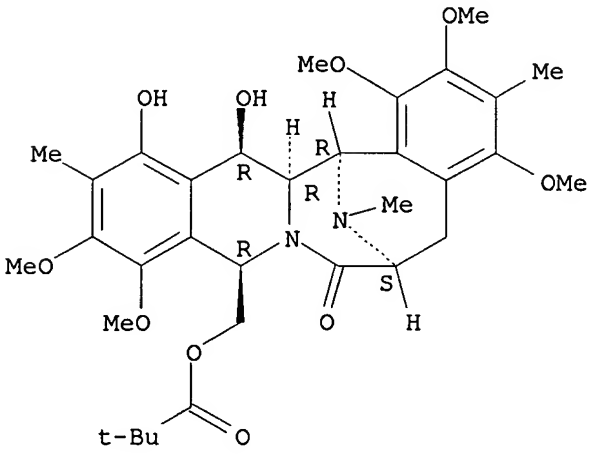
NAME)

Absolute stereochemistry.



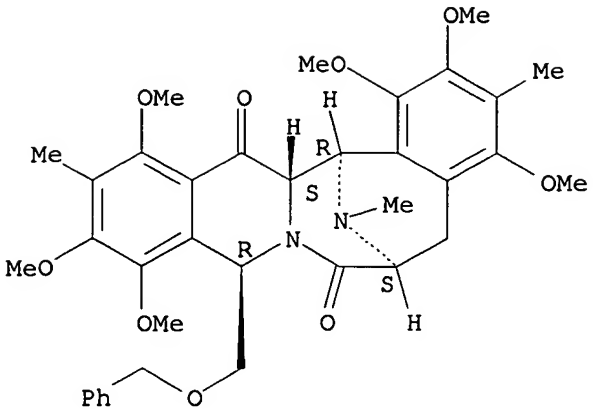
RN 351377-86-1 CAPLUS
CN Propanoic acid, 2,2-dimethyl-, [(6S,9R,14R,14aR,15R)-6,7,9,14,14a,15-hexahydro-13,14-dihydroxy-1,2,4,10,11-pentamethoxy-3,12,16-trimethyl-7-oxo-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



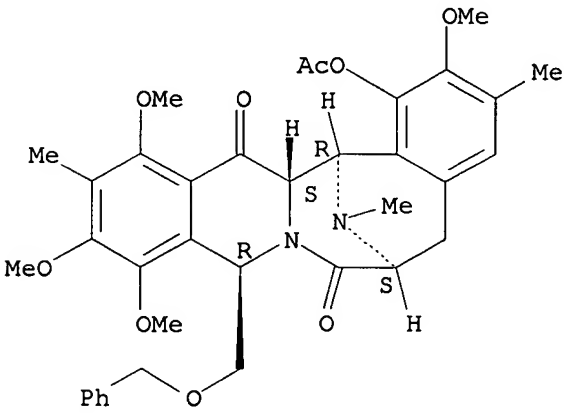
RN 351377-88-3 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 14a,15-dihydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



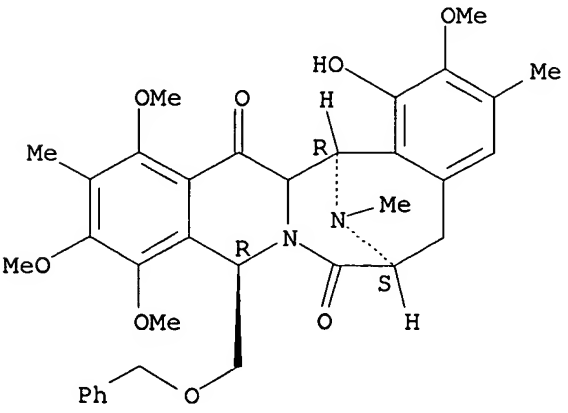
RN 351378-45-5 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 1-(acetyloxy)-14a,15-dihydro-2,10,11,13-tetramethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



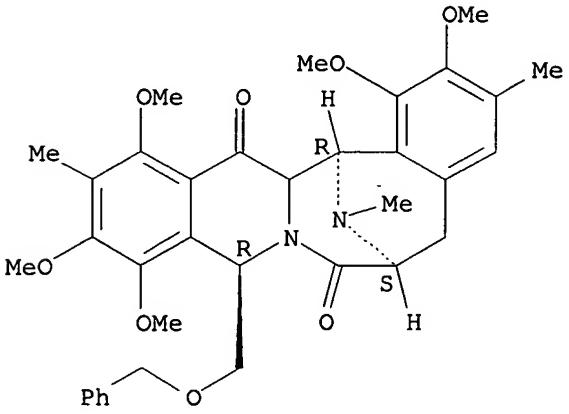
RN 351379-85-6 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 14a,15-dihydro-1-hydroxy-2,10,11,13-tetramethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



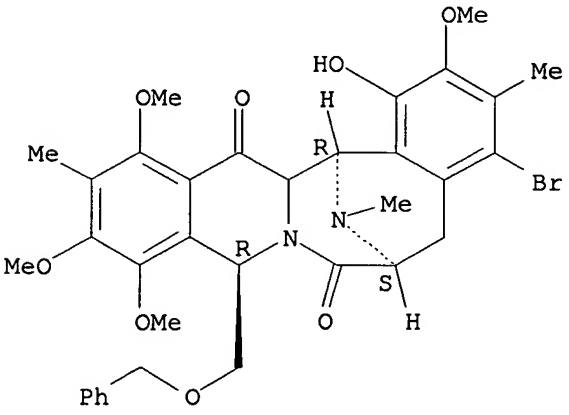
RN 351379-86-7 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 14a,15-dihydro-1,2,10,11,13-pentamethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



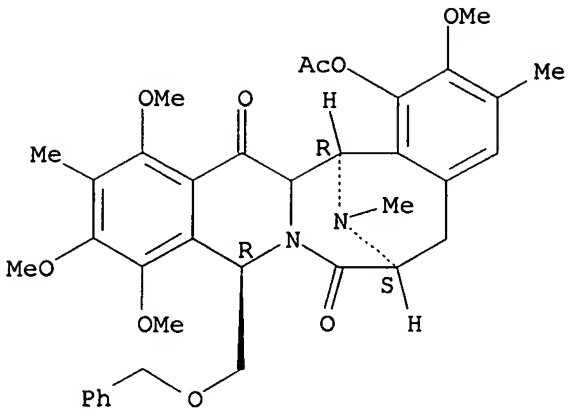
RN 351379-88-9 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 4-bromo-14a,15-dihydro-1-hydroxy-2,10,11,13-tetramethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 351379-89-0 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 1-(acetyloxy)-14a,15-dihydro-2,10,11,13-tetramethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **271578-62-2P 273720-76-6P 351377-77-0P**
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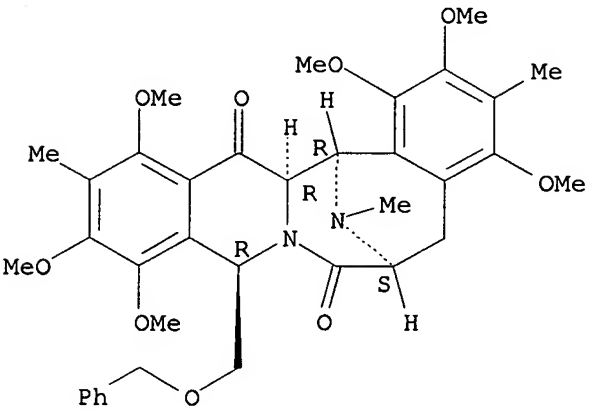
351378-24-0P 351378-26-2P 351378-28-4P
351378-30-8P 351378-32-0P 351378-43-3P
351378-57-9P 351378-78-4P 351379-71-0P
351379-73-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of saframycin-ecteinascidin analogs and their therapeutic applications)

RN 271578-62-2 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 14a,15-dihydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,14aR,15R)- (9CI) (CA INDEX NAME)

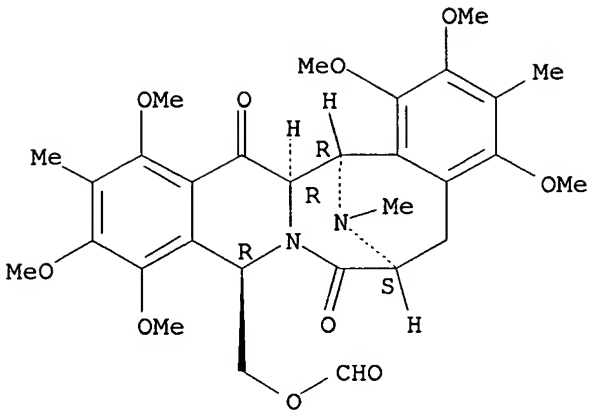
Absolute stereochemistry.



RN 273720-76-6 CAPLUS

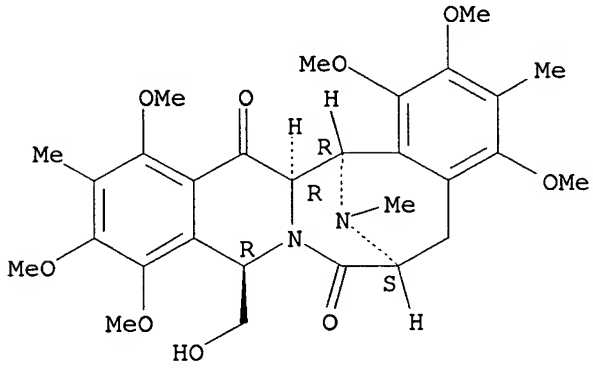
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 9-[(formyloxy)methyl]-14a,15-dihydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6S,9R,14aR,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



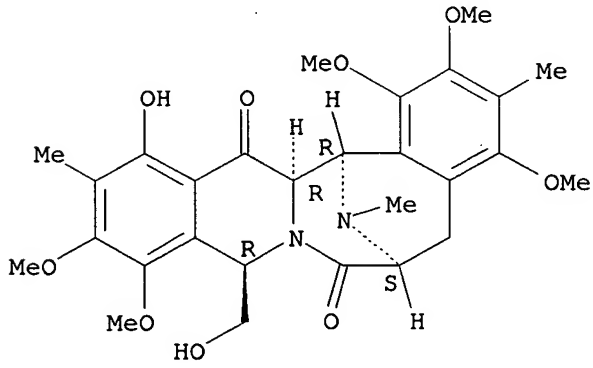
RN 351377-77-0 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 14a,15-dihydro-9-(hydroxymethyl)-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6S,9R,14aR,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



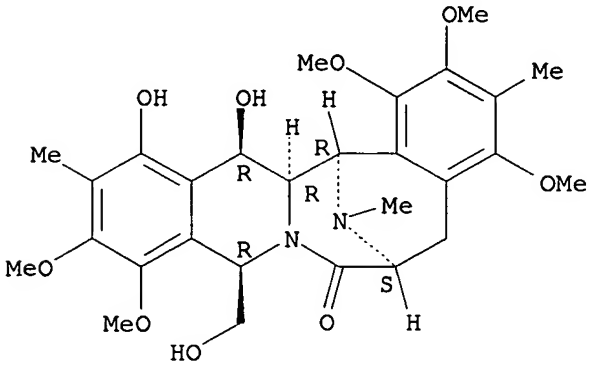
RN 351377-78-1 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 14a,15-dihydro-13-hydroxy-9-(hydroxymethyl)-1,2,4,10,11-pentamethoxy-3,12,16-trimethyl-, (6S,9R,14aR,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



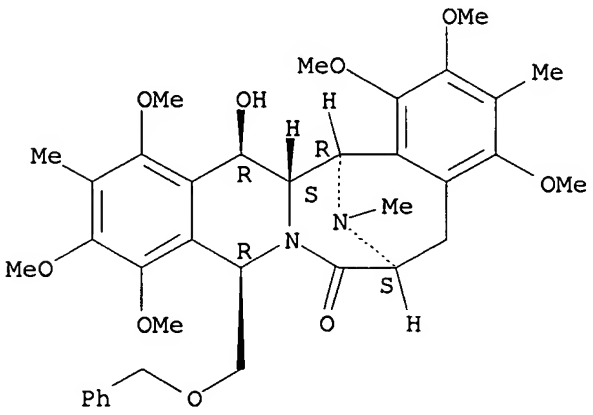
RN 351377-79-2 CAPLUS
CN 6,15-Imino-7H-isoquino[3,2-b][3]benzazocin-7-one, 5,6,9,14,14a,15-hexahydro-13,14-dihydroxy-9-(hydroxymethyl)-1,2,4,10,11-pentamethoxy-3,12,16-trimethyl-, (6S,9R,14R,14aR,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



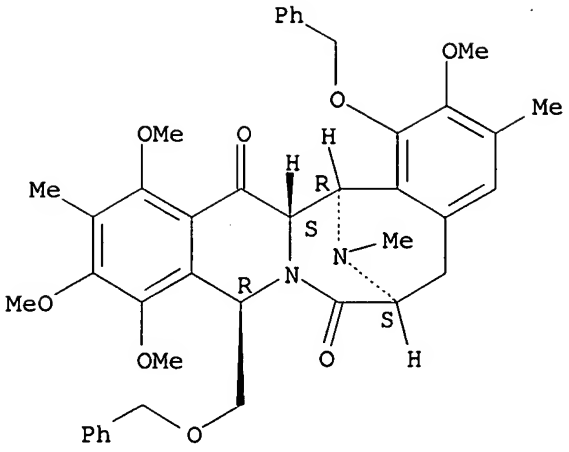
RN 351377-81-6 CAPLUS
CN 6,15-Imino-7H-isoquino[3,2-b][3]benzazocin-7-one, 5,6,9,14,14a,15-hexahydro-14-hydroxy-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,14R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



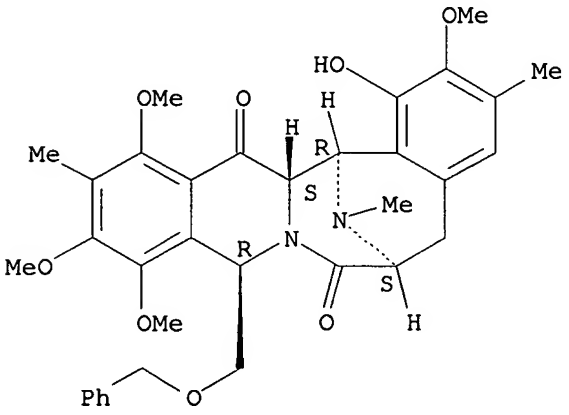
RN 351378-24-0 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 14a,15-dihydro-2,10,11,13-tetramethoxy-3,12,16-trimethyl-1-(phenylmethoxy)-9-[(phenylmethoxy)methyl]-, (6S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



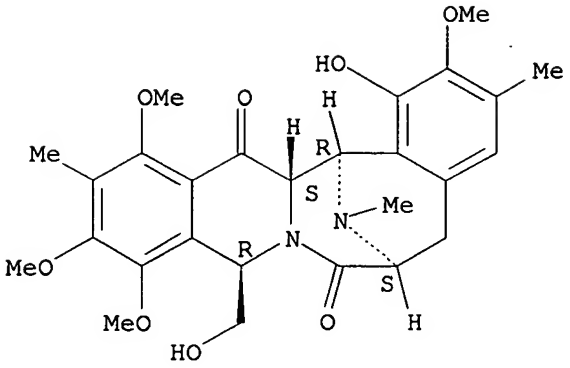
RN 351378-26-2 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 14a,15-dihydro-1-hydroxy-2,10,11,13-tetramethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



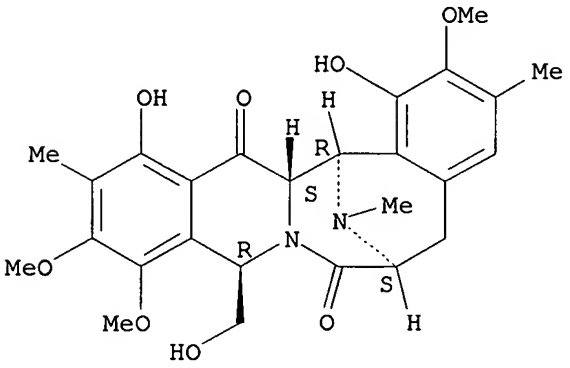
RN 351378-28-4 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 14a,15-dihydro-1-hydroxy-9-(hydroxymethyl)-2,10,11,13-tetramethoxy-3,12,16-trimethyl-, (6S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



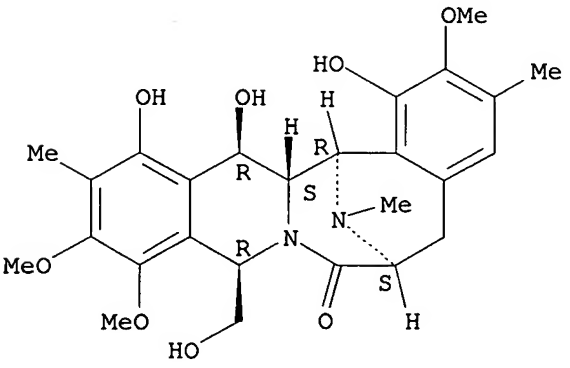
RN 351378-30-8 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 14a,15-dihydro-1,13-dihydroxy-9-(hydroxymethyl)-2,10,11-trimethoxy-3,12,16-trimethyl-, (6S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 351378-32-0 CAPLUS
CN 6,15-Imino-7H-isoquino[3,2-b][3]benzazocin-7-one, 5,6,9,14,14a,15-hexahydro-1,13,14-trihydroxy-9-(hydroxymethyl)-2,10,11-trimethoxy-3,12,16-trimethyl-, (6S,9R,14R,14aS,15R)- (9CI) (CA INDEX NAME)

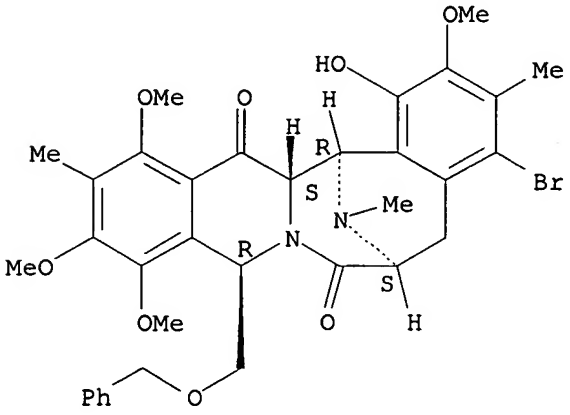
Absolute stereochemistry.



RN 351378-43-3 CAPLUS

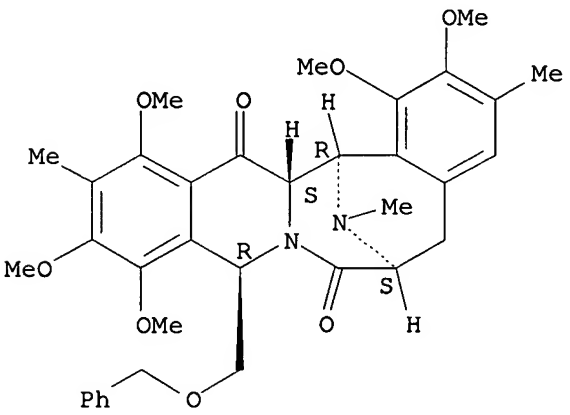
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 4-bromo-14a,15-dihydro-1-hydroxy-2,10,11,13-tetramethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 351378-57-9 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 14a,15-dihydro-1,2,10,11,13-pentamethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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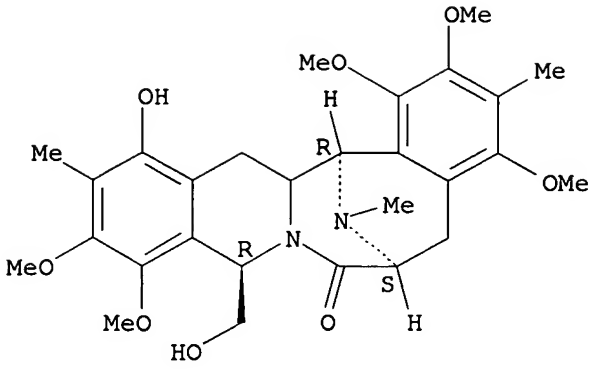
CN 6,15-Imino-7H-isoquino[3,2-b][3]benzazocin-7-one, 5,6,9,14,14a,15-hexahydro-13-hydroxy-9-(hydroxymethyl)-1,2,4,10,11-pentamethoxy-3,12,16-trimethyl-, (6S,9R,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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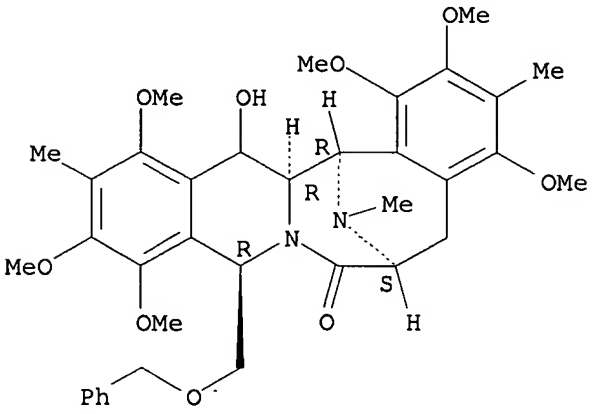
CN 6,15-Imino-7H-isoquino[3,2-b][3]benzazocin-7-one, 5,6,9,14,14a,15-hexahydro-14-hydroxy-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,14aR,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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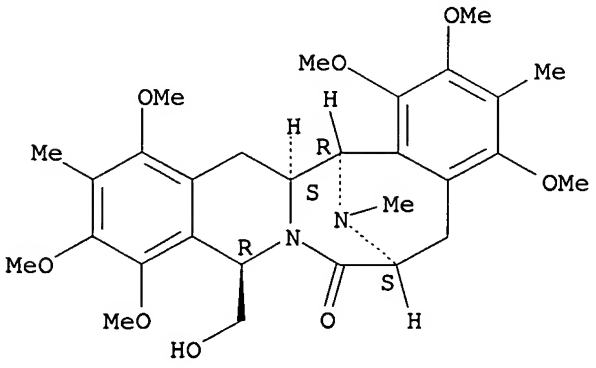
CN 6,15-Imino-7H-isoquino[3,2-b][3]benzazocin-7-one, 5,6,9,14,14a,15-hexahydro-9-(hydroxymethyl)-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 12 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:208273 CAPLUS
DOCUMENT NUMBER: 134:219960
TITLE: New antitumor marine alkaloids
INVENTOR(S): Cimino, Guido; Fontana, Angelo; Garcia Gravalos, Dolores; Wahidulla, Solimabi
PATENT ASSIGNEE(S): Instituto Biomar, S.A., Spain; Ruffles, Graham Keith
SOURCE: PCT Int. Appl., 9 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001019824	A2	20010322	WO 2000-GB3489	20000911
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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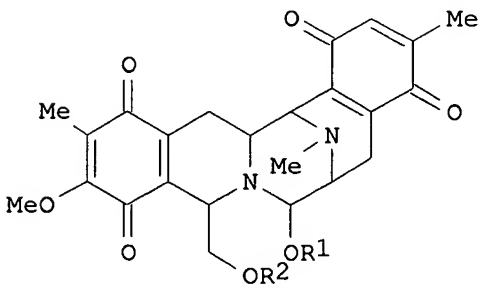
PRIORITY APPLN. INFO.:			GB 1999-21477 A	19990910
			WO 2000-GB3489 W	20000911

OTHER SOURCE(S): MARPAT 134:219960
GI



I

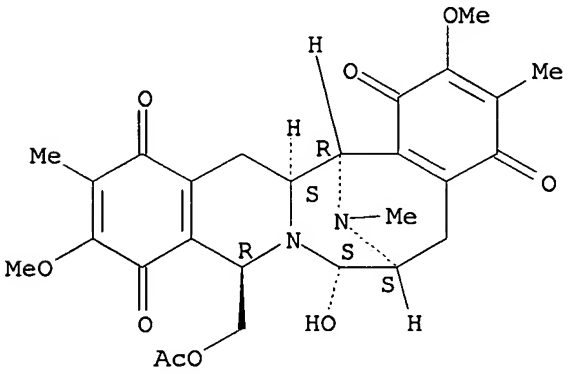
AB New antitumor alkaloids I (R1 = H, alkyl or acyl; R2 = H or acyl), which include jorumycin (I, R1 = H, R2 = acetyl), were extracted from the mollusc Jorunna funebris. The antitumor IC50 of jorumycin against P-388 tumor cells was 0.02 μM and it was also active against gram-pos. bacteria (no data).

IT **304852-37-7P**, Jorumycin
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(jorumycin antitumor alkaloid from Jorunna funebris)

RN 304852-37-7 CAPLUS

CN 6,15-Imino-4H-isoquino[3,2-b][3]benzazocine-1,4,10,13(5H)-tetrone, 9-[(acetyloxy)methyl]-6,7,9,14,14a,15-hexahydro-7-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-, (6S,7S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L7 ANSWER 13 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:645105 CAPLUS

DOCUMENT NUMBER: 133:347376

TITLE: A new antitumor isoquinoline alkaloid from the marine nudibranch Jorunna funebris

AUTHOR(S): Fontana, A.; Cavaliere, P.; Wahidulla, S.; Naik, C. G.; Cimino, G.

CORPORATE SOURCE: Istituto per la Chimica di Molecole di Interesse Biologico (ICMIB) del CNR, Arco Felice (Na), 80072, Italy

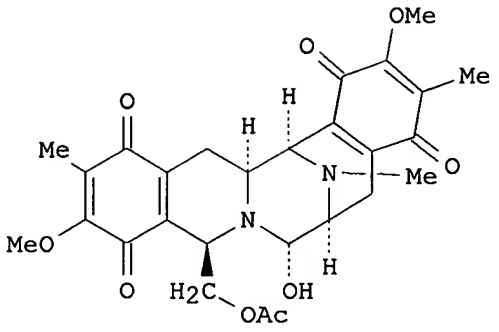
SOURCE: Tetrahedron (2000), 56(37), 7305-7308
CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

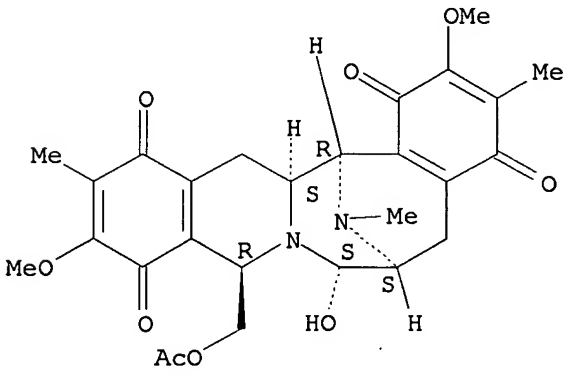
AB A new dimeric isoquinoline alkaloid, jorumycin (I), has been isolated from the skin and the mucus of the Pacific nudibranch Jorunna funebris. The structure has been fully elucidated on the grounds of ESMS data and of an extensive 2D NMR anal. The cytotoxicity of I was evaluated against various human cancer cell lines and was found to be slightly less potent than Et 743.

IT **304852-37-7P**, Jorumycine
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(antitumor isoquinoline alkaloid from marine nudibranch Jorunna funebris)

RN 304852-37-7 CAPLUS

CN 6,15-Imino-4H-isoquino[3,2-b][3]benzazocine-1,4,10,13(5H)-tetrone, 9-[(acetyloxy)methyl]-6,7,9,14,14a,15-hexahydro-7-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-, (6S,7S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 14 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

1449

ACCESSION NUMBER: 2000:248566 CAPLUS
DOCUMENT NUMBER: 133:30850
TITLE: A novel face specific Mannich closure providing access to the saframycin-ecteinascidin series of piperazine based alkaloids
AUTHOR(S): Zhou, Bishan; Guo, Jinsong; Danishefsky, Samuel J.
CORPORATE SOURCE: The Department of Chemistry, Columbia University, New

York, NY, 10027, USA
SOURCE: Tetrahedron Letters (2000), 41(13), 2043-2046
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:30850
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

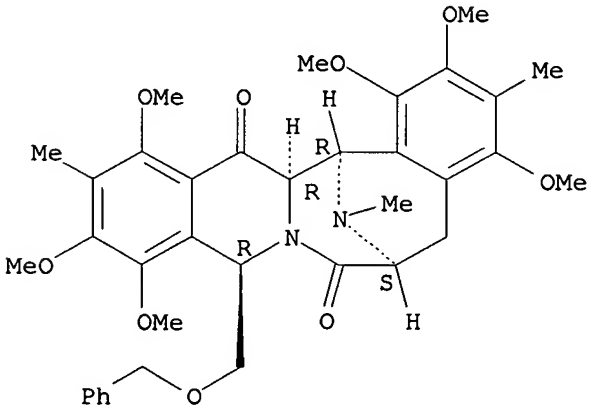
AB The Mannich-like closure of I to II directly provides the backbone stereochem. required for the titled alkaloids, in contrast to the stereochem. outcome in a related earlier case.

IT **271578-62-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(face specific Mannich closure providing access to saframycin-ecteinascidin series of piperazine based alkaloids)

RN 271578-62-2 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 14a,15-dihydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,14aR,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

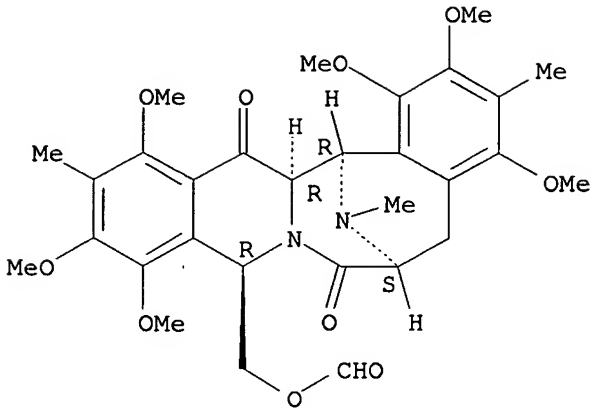


IT **273720-76-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(face specific Mannich closure providing access to saframycin-ecteinascidin series of piperazine based alkaloids)

RN 273720-76-6 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 9-[(formyloxy)methyl]-14a,15-dihydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6S,9R,14aR,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

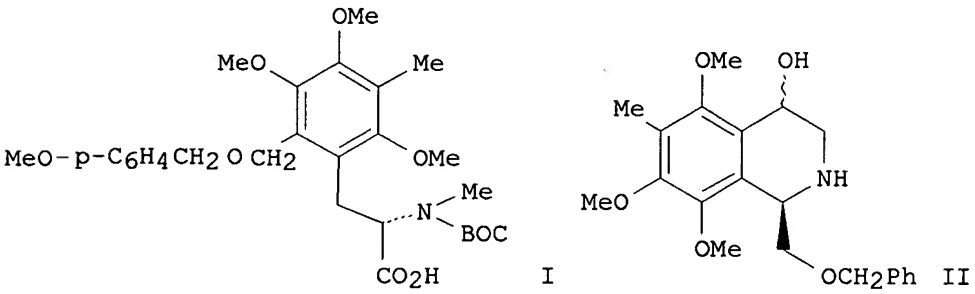


REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 15 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

1449

ACCESSION NUMBER: 2000:248565 CAPLUS
DOCUMENT NUMBER: 133:4840
TITLE: Synthetic explorations in the saframycin-ecteinascidin series: construction of major chiral subunits through catalytic asymmetric induction
AUTHOR(S): Zhou, Bishan; Edmondson, Scott; Padron, Juan; Danishefsky, Samuel J.
CORPORATE SOURCE: The Department of Chemistry, Columbia University, New York, NY, 10027, USA
SOURCE: Tetrahedron Letters (2000), 41(13), 2039-2042
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:4840
GI



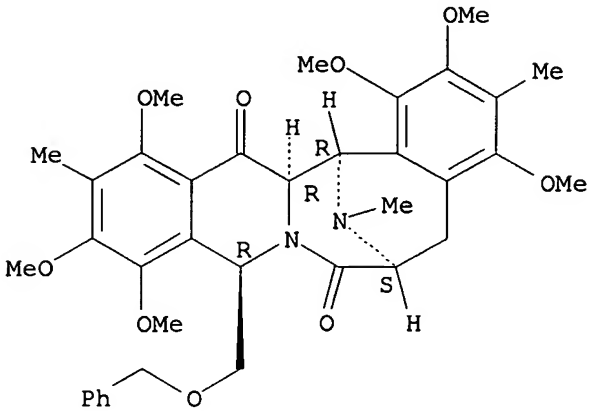
AB The major subunits (I and II) needed to reach the titled targets have been assembled by chemical, which included p-Claisen rearrangement, asym. epoxidn. and asym. dihydroxylation.

IT **271578-62-2P**
RL: PNU (Preparation, unclassified); PREP (Preparation)
(construction of major chiral saframycin subunits via catalytic asym. induction)

RN 271578-62-2 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione,

14a,15-dihydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,14aR,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 16 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

1409

ACCESSION NUMBER: 1995:717839 CAPLUS
DOCUMENT NUMBER: 123:227861
TITLE: Synthesis of saframycins. XI. Synthetic studies toward a total synthesis of safracin A
AUTHOR(S): Saito, Naoki; Harada, Shunji; Yamashita, Mihoko; Saito, Takeshi; Yamaguchi, Kentaro; Kubo, Akinori
CORPORATE SOURCE: Meiji Coll. Pharmacy, Tokyo, 154, Japan
SOURCE: Tetrahedron (1995), 51(30), 8213-30
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Pergamon
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:227861
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

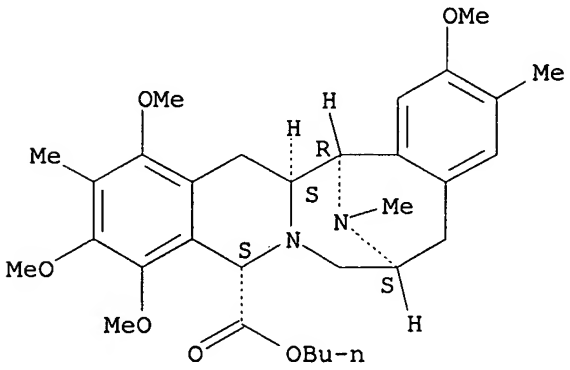
AB A synthetic strategy for the preparation of the isoquinolinequinone antibiotic safracin A is outlined. The authors' initial strategy for the construction of the ABC ring was based on a retrosynthetic anal. Conversion of piperazinedione I in five steps to the imide was followed by a 1,2-reduction with lithium tri-tert-butoxyaluminum hydride to give the allylic alc. II. This compound was then cyclized to the 1,5-imino-3-benzazocine III (R = CO2CHMe2) and an unwanted indeno[1,2-b]pyrazin-2-one. Conversion of III (R = H) to the pentacyclic pyruvamide IV was completed in a nine step sequence. Finally, IV was subjected to a two-step oxidative demethylation to provide the quinones V (R1 = Me, R2 = H; R1 = H, R2 = NO2). An unsuccessful attempt to introduce a hydroxyl group into the C-1 position of the quinones V is also described.

IT **168132-84-1P 168132-86-3P 168254-07-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(synthetic studies toward total synthesis of safracin A)

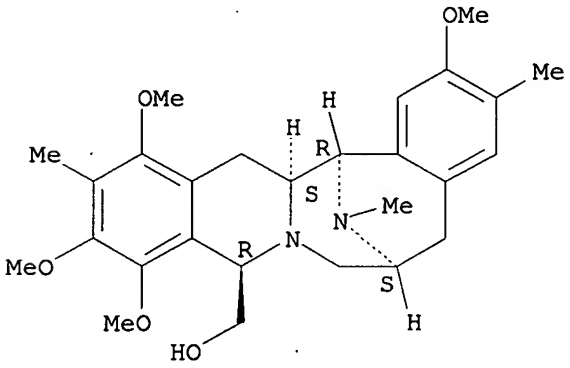
RN 168132-84-1 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid, 6,7,9,14,14a,15-hexahydro-2,10,11,13-tetramethoxy-3,12,16-trimethyl-, butyl ester, (6α,9α,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



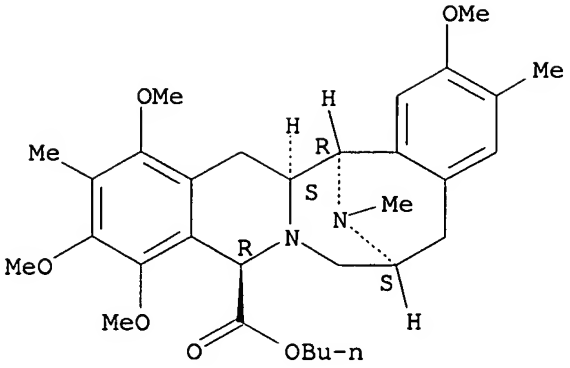
RN 168132-86-3 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol, 6,7,9,14,14a,15-hexahydro-2,10,11,13-tetramethoxy-3,12,16-trimethyl-, (6α,9β,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



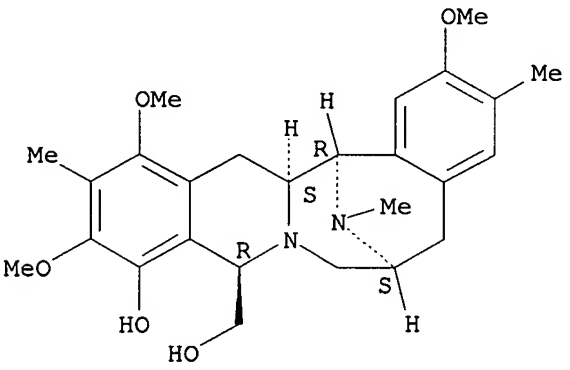
RN 168254-07-7 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid, 6,7,9,14,14a,15-hexahydro-2,10,11,13-tetramethoxy-3,12,16-trimethyl-, butyl ester, (6α,9β,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



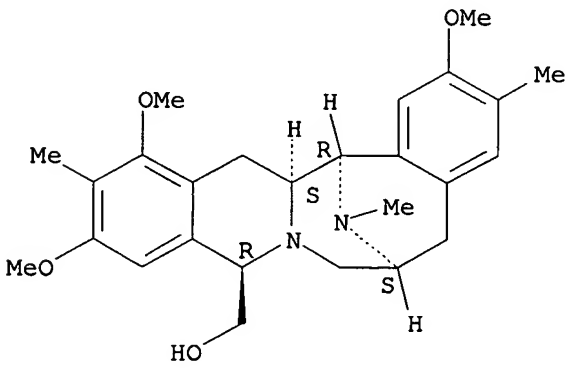
IT **168132-87-4P 168132-88-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthetic studies toward total synthesis of safracin A)
RN 168132-87-4 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol, 6,7,9,14,14a,15-hexahydro-10-hydroxy-2,11,13-trimethoxy-3,12,16-trimethyl-, (6α,9β,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



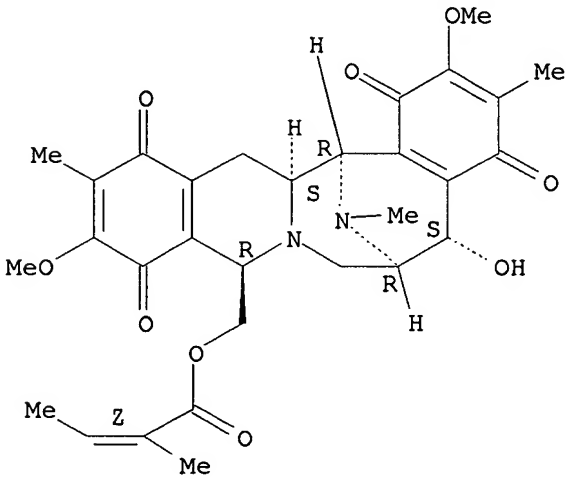
RN 168132-88-5 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol, 6,7,9,14,14a,15-hexahydro-2,11,13-trimethoxy-3,12,16-trimethyl-, (6α,9β,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



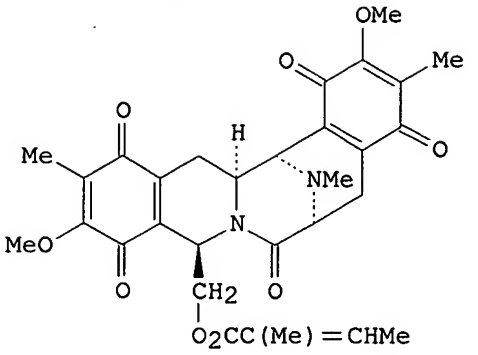
L7 ANSWER 17 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1994:298315 CAPLUS
DOCUMENT NUMBER: 120:298315
TITLE: A stereocontrolled total synthesis of (±)-renieramycin A
AUTHOR(S): Linton, Steven Douglas
CORPORATE SOURCE: Rice Univ., Houston, TX, USA
SOURCE: (1992) 149 pp. Avail.: Univ. Microfilms Int., Order No. DA9234382
From: Diss. Abstr. Int. B 1993, 53(7), 3485
DOCUMENT TYPE: Dissertation
LANGUAGE: English
AB Unavailable
IT **132342-06-4P**, (±)-Renieramycin A
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(stereocontrolled total synthesis of)
RN 132342-06-4 CAPLUS
CN 2-Butenoic acid, 2-methyl-, (1,5,6,7,9,10,13,14,14a,15-decahydro-5-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl)methyl ester, [5α,6α,9β(Z),14aα,15α]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



L7 ANSWER 18 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1992:547449 CAPLUS
DOCUMENT NUMBER: 117:147449
TITLE: Renieramycin G, a new alkaloid from the sponge Xestospongia caycedoi
AUTHOR(S): Davidson, Bradley S.
CORPORATE SOURCE: Dep. Chem., Univ. Hawaii, Honolulu, HI, 96822, USA
SOURCE: Tetrahedron Letters (1992), 33(26), 3721-4
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

1449



I

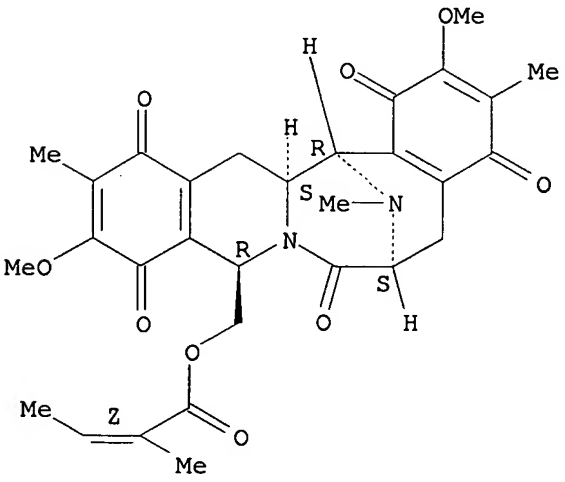
AB A new cytotoxic alkaloid, renieramycin G (I), was isolated, along with previously reported metabolites mimosamycin, renierol, and N-formyl-1,2-dihydrorenierone, from the Fijian sponge X. caycedoi. The structure of renieramycin G was deduced from spectral data.

IT **143458-75-7**, Renieramycin G
RL: BIOL (Biological study)
(from Xestospongia caycedoi, structure of)

RN 143458-75-7 CAPLUS

CN 2-Butenoic acid, 2-methyl-, (1,5,6,7,9,10,13,14,14a,15-decahydro-2,11-dimethoxy-3,12,16-trimethyl-1,4,7,10,13-pentaoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl)methyl ester, [6S-[6α,9β(Z),14aα,15α]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L7 ANSWER 19 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1991:608305 CAPLUS

DOCUMENT NUMBER: 115:208305

TITLE: Synthesis of saframycins. VII. The synthesis of novel renieramycin congeners

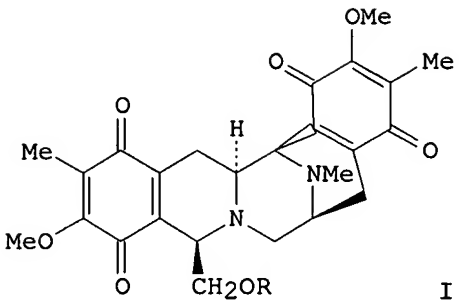
AUTHOR(S): Saito, Naoki; Yamauchi, Reiko; Kubo, Akinori

CORPORATE SOURCE: Meiji Coll. Pharm., Tokyo, 154, Japan

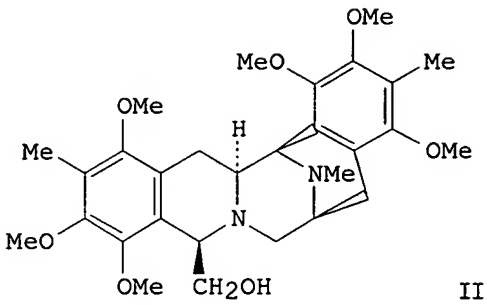
SOURCE: Heterocycles (1991), 32(6), 1203-14

1449

CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 115:208305
GI



I

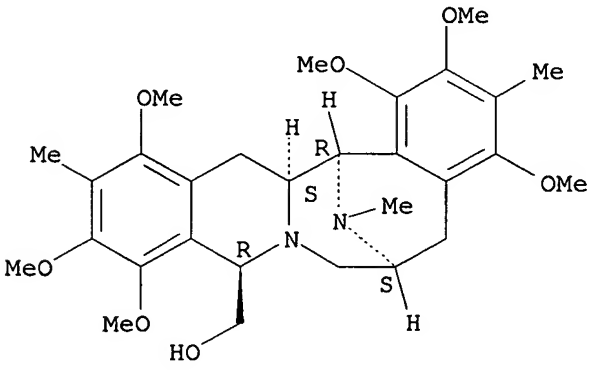


II

AB The marine alkaloid renieramycin congeners I (R = H, Ac, EtCO) were synthesized starting from the alc. II which was the key intermediate for saframycin B synthesis.

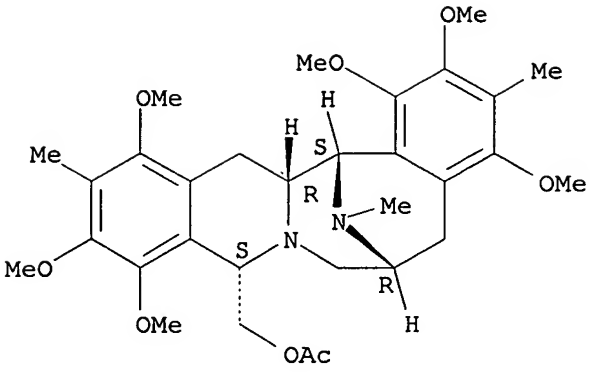
IT **112446-04-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation of)
RN 112446-04-5 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6α,9β,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



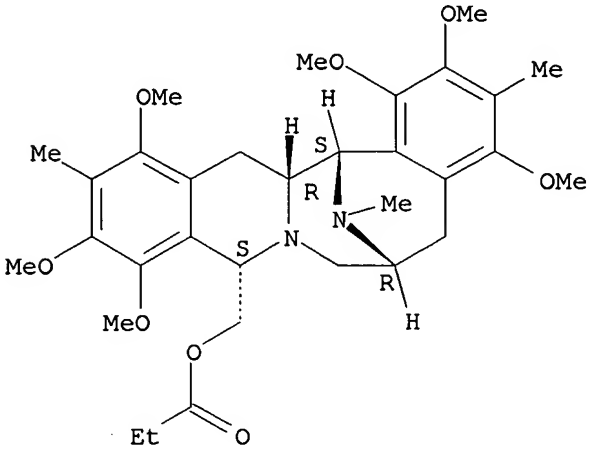
IT **112995-91-2P 136581-76-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and demethylation of)
RN 112995-91-2 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, acetate (ester), (6α,9β,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



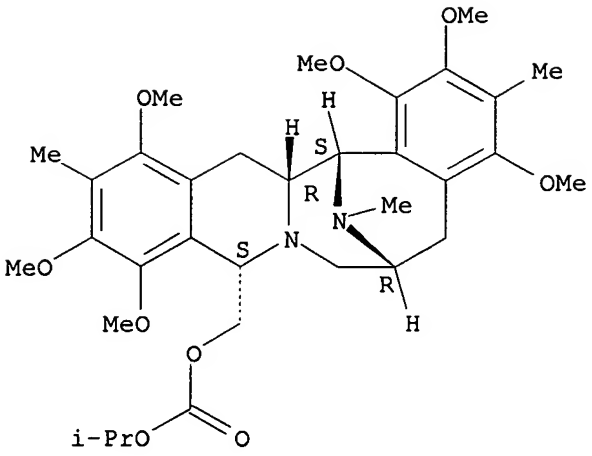
RN 136581-76-5 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, propanoate (ester), (6α,9β,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



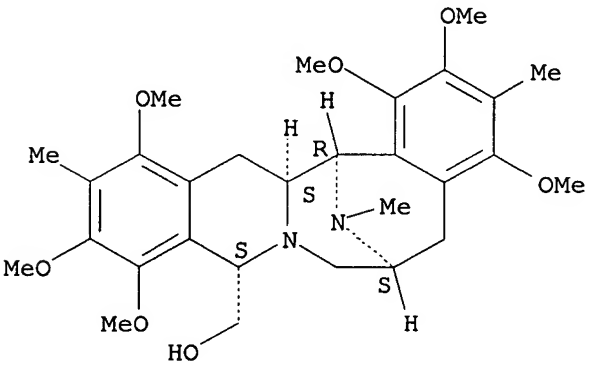
IT **136604-12-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 136604-12-1 CAPLUS
CN Carbonic acid, (6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl 1-methylethyl ester, (6α,9β,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

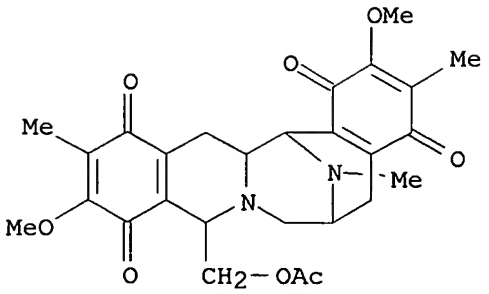


IT **112529-59-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with phthalimide)
RN 112529-59-6 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6α,9α,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

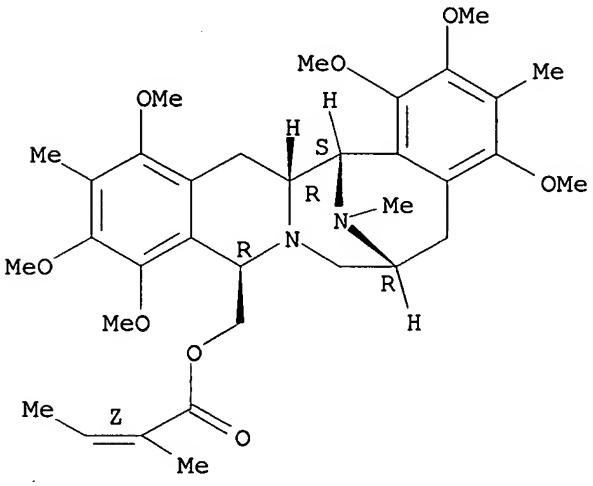


IT **112995-93-4P 136581-72-1P 136581-74-3P 136581-77-6P 136656-91-2P 136656-92-3P 136656-93-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 112995-93-4 CAPLUS
CN 6,15-Imino-4H-isoquino[3,2-b][3]benzazocine-1,4,10,13(9H)-tetrone, 9-[(acetyloxy)methyl]-5,6,7,14,14a,15-hexahydro-2,11-dimethoxy-3,12,16-trimethyl-, (6α,9β,14aα,15α)- (9CI) (CA INDEX NAME)



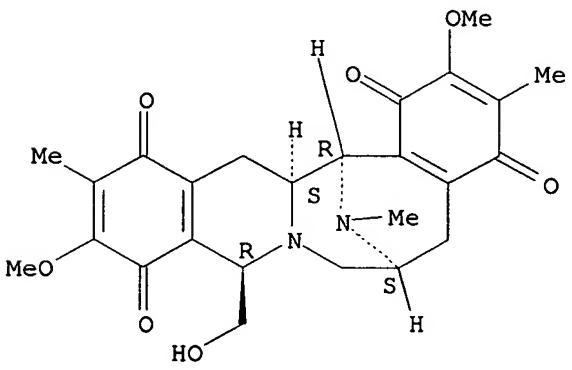
RN 136581-72-1 CAPLUS
CN 2-Butenoic acid, 2-methyl-, (6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl ester, [6α,9α(Z),14aα,15α]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.

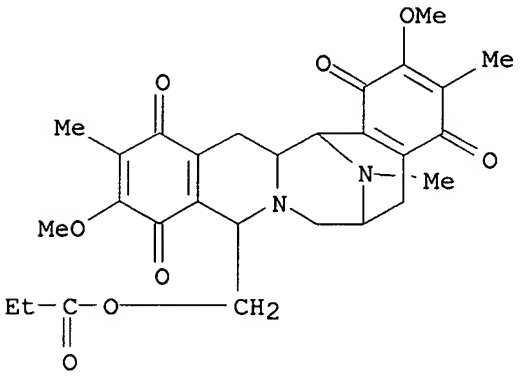


RN 136581-74-3 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-1,4,10,13-tetrone, 6,7,9,14,14a,15-hexahydro-9-(hydroxymethyl)-2,11-dimethoxy-3,12,16-trimethyl-, (6R,9S,14aR,15S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

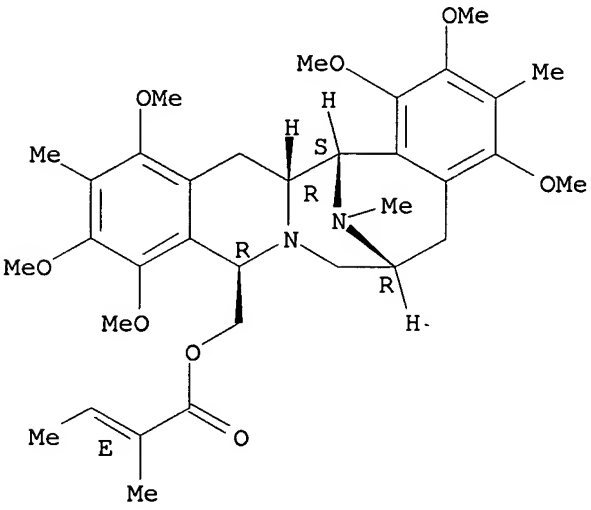


RN 136581-77-6 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-1,4,10,13-tetrone, 6,7,9,14,14a,15-hexahydro-2,11-dimethoxy-3,12,16-trimethyl-9-[(1-oxopropoxy)methyl]-, (6α,9β,14aα,15α)- (9CI) (CA INDEX NAME)



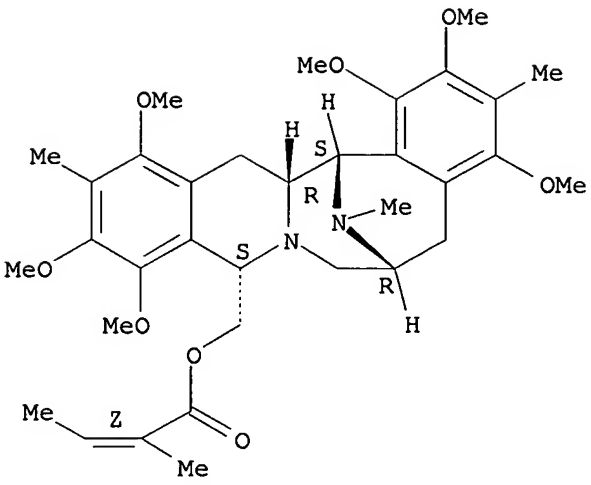
RN 136656-91-2 CAPLUS
CN 2-Butenoic acid, 2-methyl-, (6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl ester, [6α,9α(E),14aα,15α]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



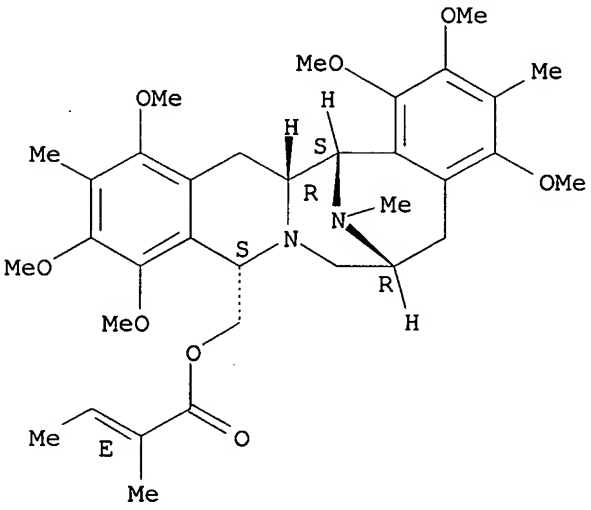
RN 136656-92-3 CAPLUS
CN 2-Butenoic acid, 2-methyl-, (6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl ester, [6α,9β(Z),14aα,15α]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



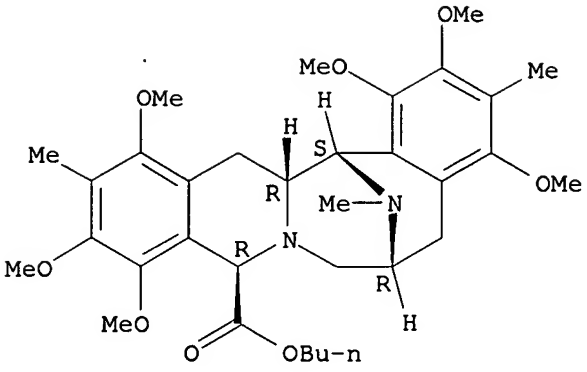
RN 136656-93-4 CAPLUS
CN 2-Butenoic acid, 2-methyl-, (6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl ester, [6α,9β(E),14aα,15α]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



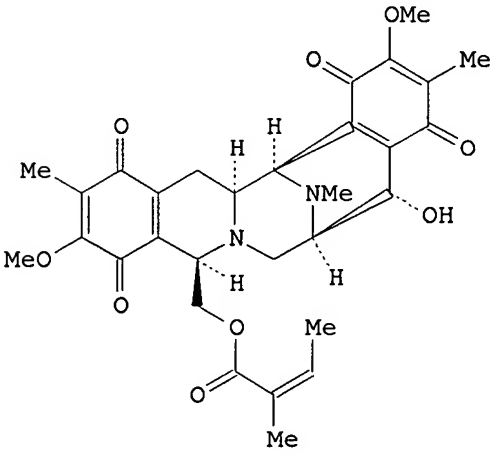
IT **112529-58-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of)
RN 112529-58-5 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, butyl ester, (6α,9α,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



1449

L7 ANSWER 20 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1991:102523 CAPLUS
DOCUMENT NUMBER: 114:102523
TITLE: A stereocontrolled total synthesis of (±)-renieramycin A
AUTHOR(S): Fukuyama, Tohru; Linton, Steven D.; Tun, Min Min
CORPORATE SOURCE: Dep. Chem., Rice Univ., Houston, TX, 77251, USA
SOURCE: Tetrahedron Letters (1990), 31(42), 5989-92
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



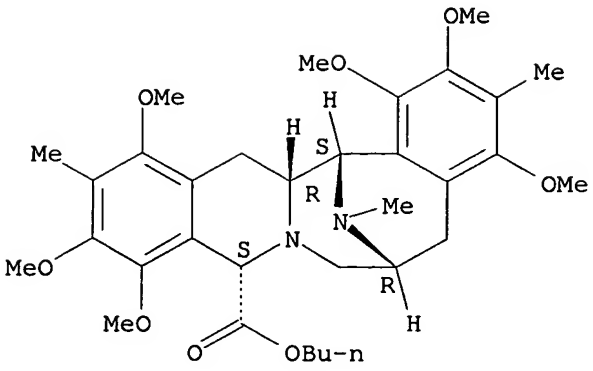
I

AB The first total synthesis of (±)-renieramycin A (I) is described. The stereochem. of the angelate side chain was unequivocally determined by X-ray crystallog. anal. of the penultimate intermediate.

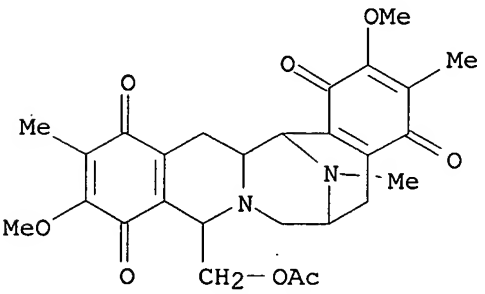
IT **132340-98-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 132340-98-8 CAPLUS

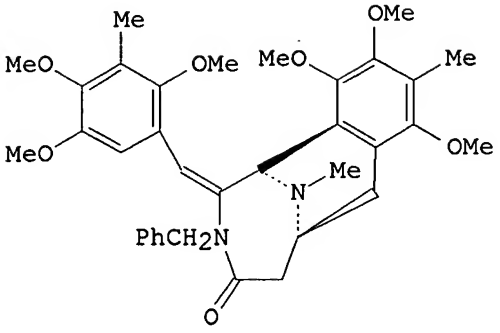
CN 2-Butenoic acid, 2-methyl-, (6,7,9,14,14a,15-hexahydro-1,5,10-trihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl ester, [5α,6α,9α(Z),14a.alph a.,15α]- (9CI) (CA INDEX NAME)



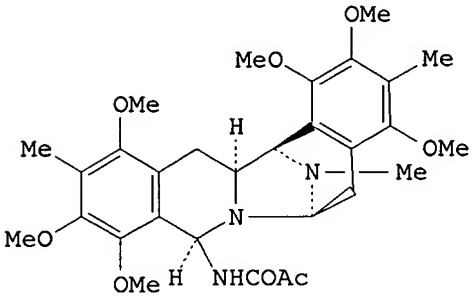
IT **112995-93-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 112995-93-4 CAPLUS
CN 6,15-Imino-4H-isoquino[3,2-b][3]benzazocine-1,4,10,13(9H)-tetrone, 9-[(acetyloxy)methyl]-5,6,7,14,14a,15-hexahydro-2,11-dimethoxy-3,12,16-trimethyl-, (6α,9β,14aα,15α)- (9CI) (CA INDEX NAME)



L7 ANSWER 25 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1988:55713 CAPLUS
DOCUMENT NUMBER: 108:55713
TITLE: Studies on the total synthesis of saframycin B
AUTHOR(S): Kobo, Akiyoshi; Saito, Naoki; Yamato, Hidekazu; Nakamura, Madoka
CORPORATE SOURCE: Meiji Coll. Pharm., Japan
SOURCE: Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1986), 28th, 465-72
CODEN: TYKYDS
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
GI



II



III

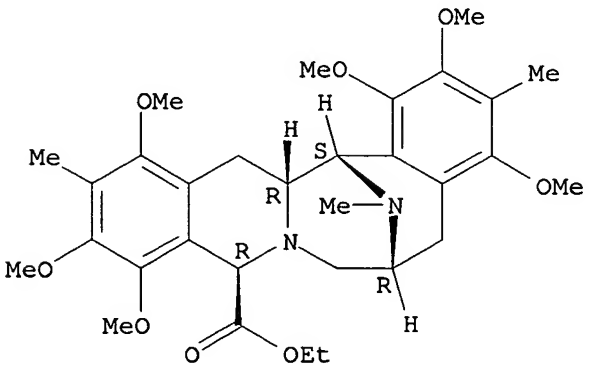
AB Saframycin B (I) which is an antitumor antibiotic, produced by Streptomyces lavendulae were prepared The preparation of safaramycin B intermediate II was reviewed. II was converted into the pentacyclic compound III in 10 steps. Oxidation of III with 10N HNO3 afforded I in 1% yield. The yield of I was raised to 41% by treatment with BBr3 at -78° followed by 10N HNO3.

IT **112446-10-3P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)

RN 112446-10-3 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, ethyl ester, (6α,9α,14aα,15α)- (9CI) (CA INDEX NAME)

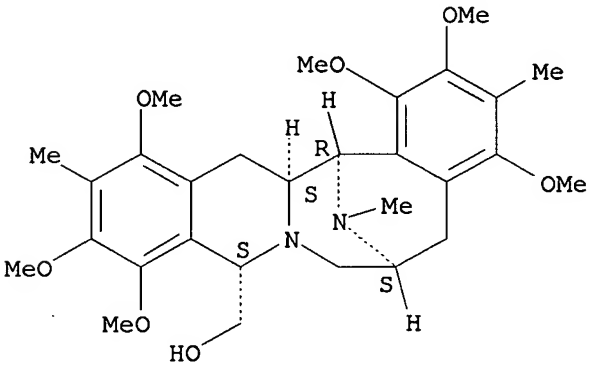
Relative stereochemistry.



IT **112529-59-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

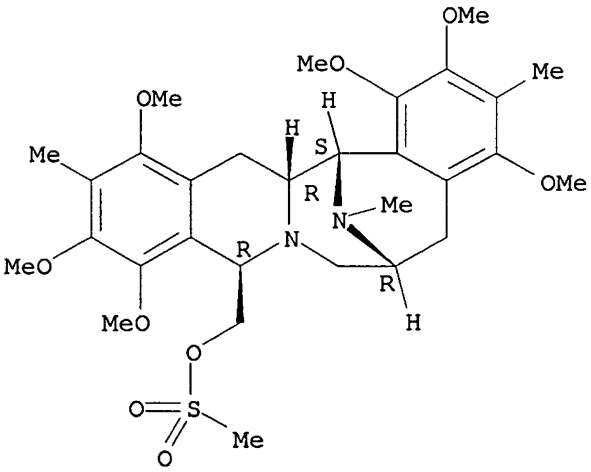
(Reactant or reagent)
(preparation and methylation of)
RN 112529-59-6 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6α,9α,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT **112446-11-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with azide)
RN 112446-11-4 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, methanesulfonate (ester), (6α,9α,14aα,15α)- (9CI) (CA INDEX NAME)

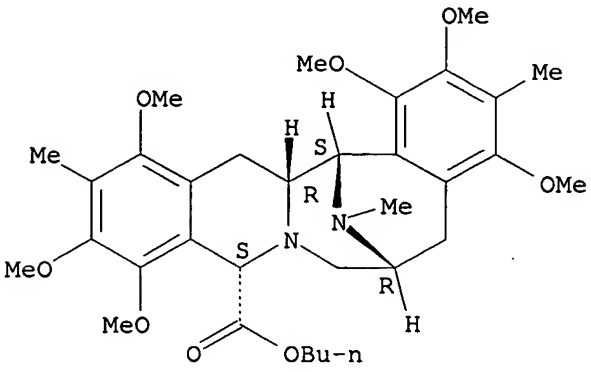
Relative stereochemistry.



IT **112446-05-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 112446-05-6 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid,

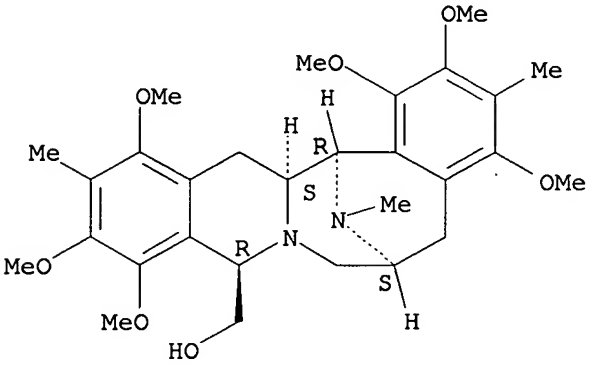
6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, butyl ester, (6α,9β,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



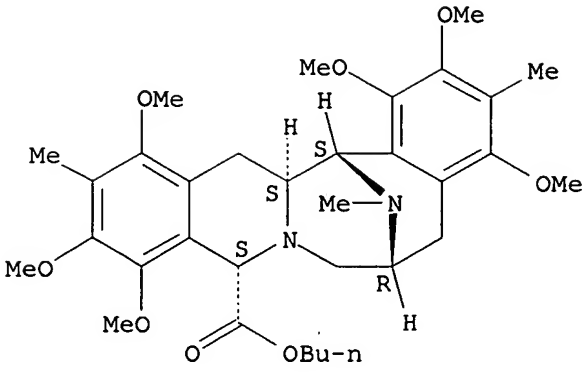
IT **112446-04-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, reaction with phthalimide, hydrazinolysis, and acylation of)
RN 112446-04-5 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6α,9β,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



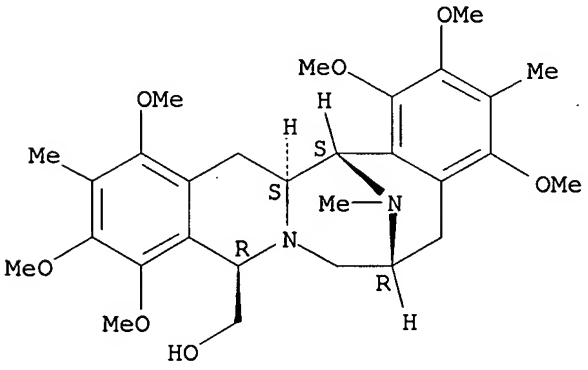
IT **112529-58-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, reduction, and isomerization of)
RN 112529-58-5 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, butyl ester, (6α,9α,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



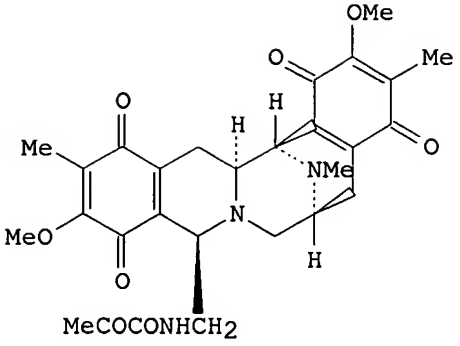
IT **115510-13-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for saframycin B)
RN 115510-13-9 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, [6R-(6α,9α,14aβ,15α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

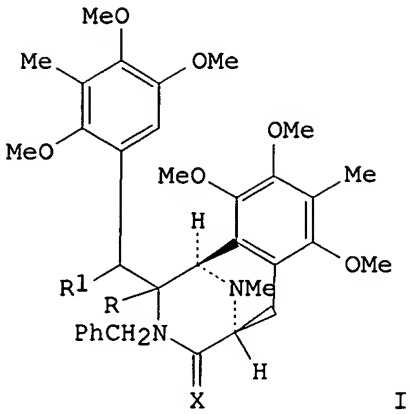


L7 ANSWER 24 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1988:112030 CAPLUS
DOCUMENT NUMBER: 108:112030
TITLE: Synthesis of saframycins. I. Total synthesis of (±)-saframycin B and its congeners
AUTHOR(S): Kubo, Akinori; Saito, Naoki; Yamauchi, Reiko; Sakai, Shinichiro
CORPORATE SOURCE: Meiji Coll. Pharm., Tokyo, 154, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1987), 35(5), 2158-61
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 108:112030
GI

1449



I



II

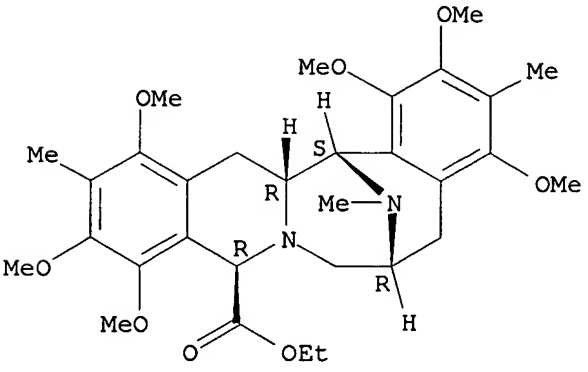
AB The total synthesis of saframycin B (I) was achieved from tricyclic lactam II (RR1 = bond; X = O). The key step is the stereoselective intramol. cyclization of the amino acetal II (R = R1 = H; X = H2). The structure of a pentacyclic intermediate was confirmed by x-ray crystallog.

IT **112446-10-3P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)

RN 112446-10-3 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, ethyl ester, (6α,9α,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

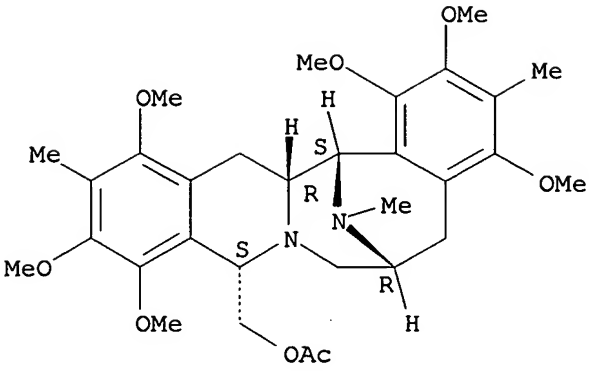


IT **112995-91-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and demethylation of)

RN 112995-91-2 CAPLUS

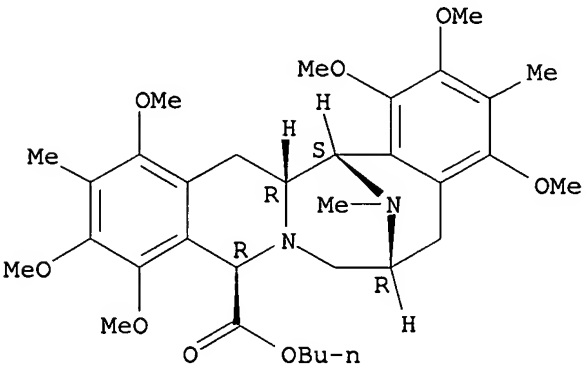
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, acetate (ester), (6α,9β,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



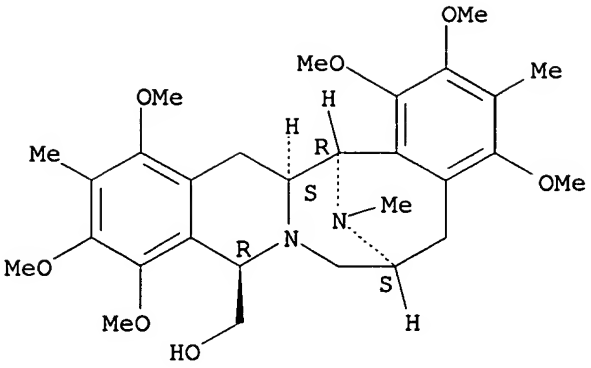
IT **112529-58-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and epimerization of)
RN 112529-58-5 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, butyl ester, (6α,9α,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



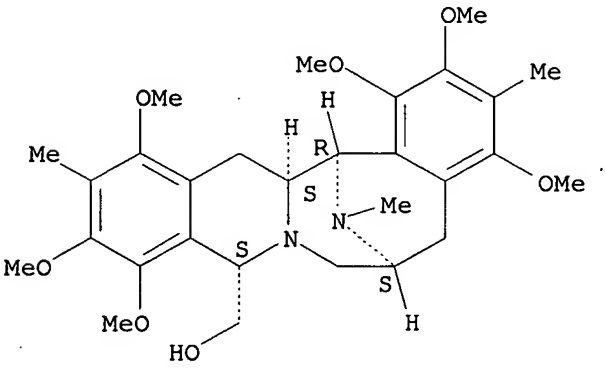
IT **112446-04-5P 112529-59-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with phthalimide)
RN 112446-04-5 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6α,9β,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 112529-59-6 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6α,9α,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT **112446-05-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 112446-05-6 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, butyl ester, (6α,9β,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

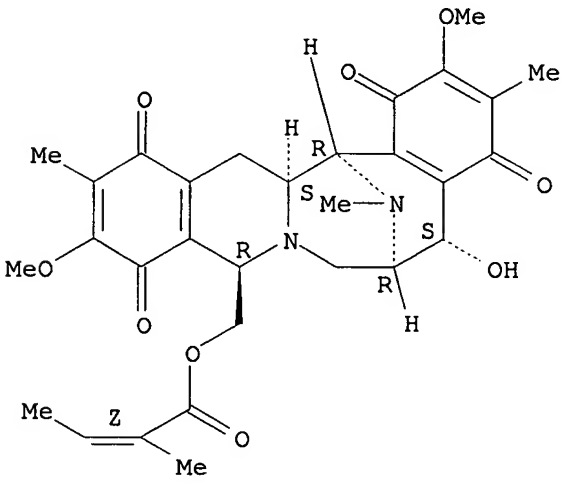
the first naturally occurring isoindole to be described, was confirmed by an unambiguous synthesis. The structures of the renieramycins were determined by anal. of spectral data, especially 1H NMR. All the compds. showed antimicrobial activity.

IT **79664-60-1 79664-61-2 79664-62-3 79664-63-4**
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); BIOL (Biological study); OCCU (Occurrence)
(of sponge)

RN 79664-60-1 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(5S,6R,9R,14aS,15R)-1,5,6,7,9,10,13,14,14a,15-decahydro-5-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

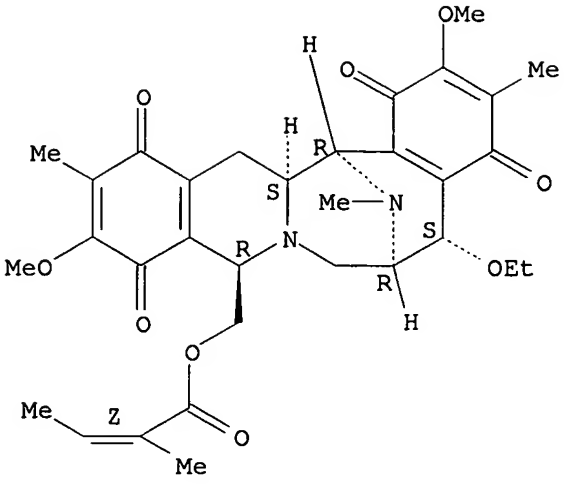
Absolute stereochemistry.
Double bond geometry as shown.



RN 79664-61-2 CAPLUS

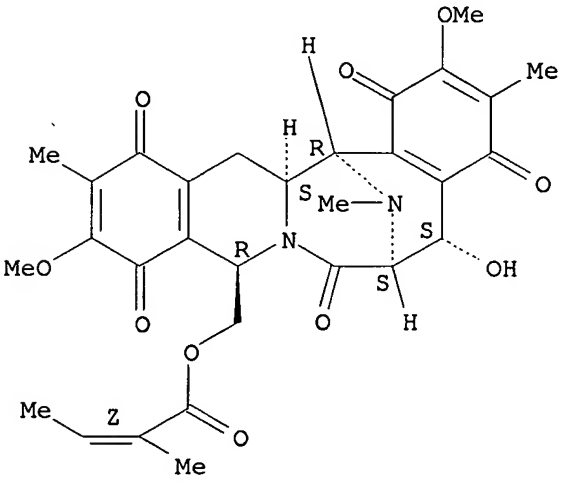
CN 2-Butenoic acid, 2-methyl-, [(5S,6R,9R,14aS,15R)-5-ethoxy-1,5,6,7,9,10,13,14,14a,15-decahydro-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



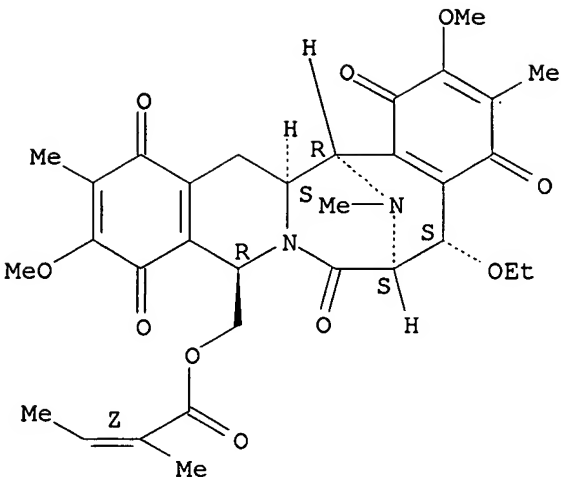
RN 79664-62-3 CAPLUS
CN 2-Butenoic acid, 2-methyl-, [(5S,6S,9R,14aS,15R)-1,5,6,7,9,10,13,14,14a,15-decahydro-5-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-1,4,7,10,13-pentaoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 79664-63-4 CAPLUS
CN 2-Butenoic acid, 2-methyl-, [(5S,6S,9R,14aS,15R)-5-ethoxy-1,5,6,7,9,10,13,14,14a,15-decahydro-2,11-dimethoxy-3,12,16-trimethyl-1,4,7,10,13-pentaoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.


OMe
H
O
Me
O
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R
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MeO
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OEt
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Me

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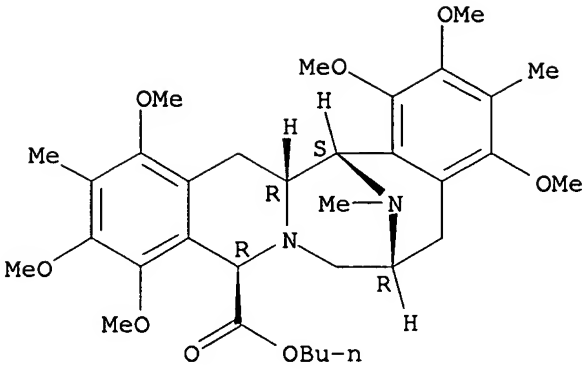
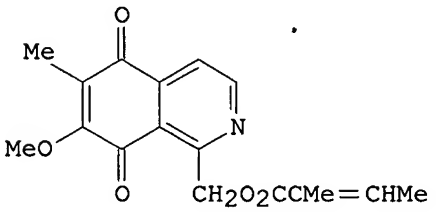
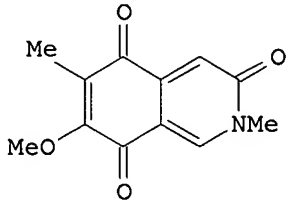


L7 ANSWER 26 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

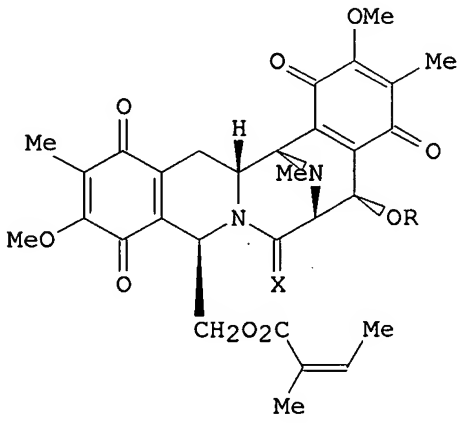
ACCESSION NUMBER: 1982:31904 CAPLUS
DOCUMENT NUMBER: 96:31904
TITLE: Antimicrobial metabolites of the sponge Reniera sp
AUTHOR(S): Frincke, James M.; Faulkner, D. John
CORPORATE SOURCE: Scripps Inst. Oceanogr., La Jolla, CA, 92093, USA
SOURCE: Journal of the American Chemical Society (1982), 104(1), 265-9
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



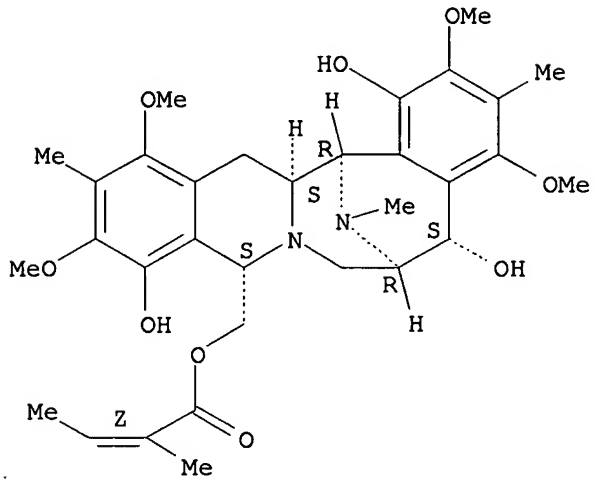
II



IV, R=H, X=2H
V, R=Et, X=2H
VI, R=H, X=O
VII, R=Et, X=O

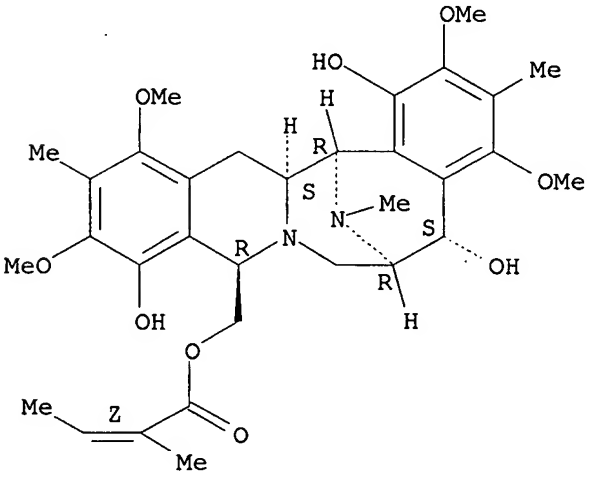
AB The sponge Reniera contains renierone (I), mimosamycin (II), N-formyl-1,2-dihydrorenierone, O-demethylrenierone, 1,6-dimethyl-7-methoxy-5,8-dihydroisoquinoline-5,8-dione, 2,5-dimethyl-6-methoxy-4,7-dihydroisoindole-4,7-dione (III), and renieramycins A-D (IV-VII). III,

Relative stereochemistry.
Double bond geometry as shown.



IT **132277-62-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, crystal structure, and oxidation of)
RN 132277-62-4 CAPLUS
CN 2-Butenoic acid, 2-methyl-, (6,7,9,14,14a,15-hexahydro-1,5,10-trihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl ester, [5α,6α,9β(Z),14a.alpha.,15α]- (9CI) (CA INDEX NAME)

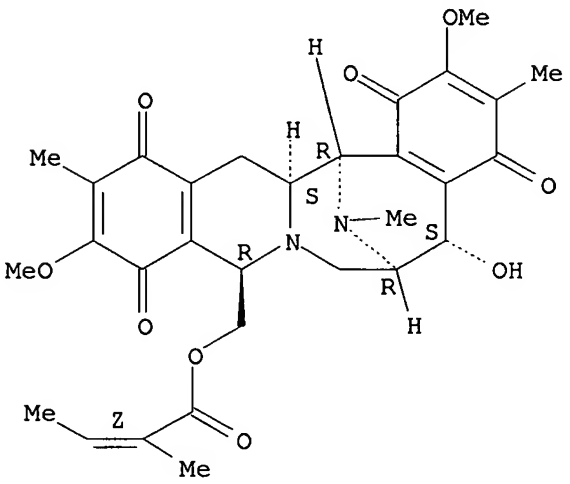
Relative stereochemistry.
Double bond geometry as shown.



IT **132342-06-4P**, (±)-Renieramycin A
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(stereocontrolled total synthesis of)
RN 132342-06-4 CAPLUS
CN 2-Butenoic acid, 2-methyl-, (1,5,6,7,9,10,13,14,14a,15-decahydro-5-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-

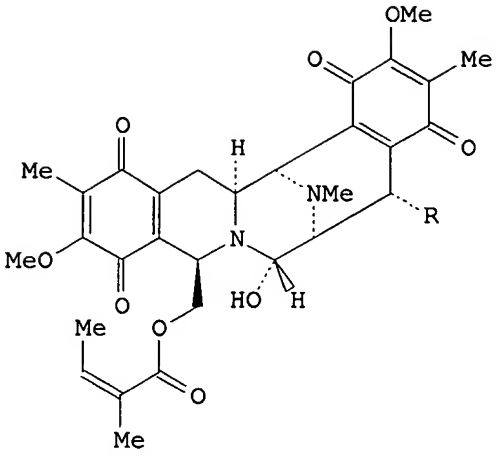
isoquino[3,2-b][3]benzazocin-9-yl)methyl ester, [5α,6α,9β(Z),14aα,15α]- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



L7 ANSWER 21 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:	1990:4919 CAPLUS
DOCUMENT NUMBER:	112:4919
TITLE:	Renieramycins E and F from the sponge Reniera sp.: reassignment of the stereochemistry of the renieramycins
AUTHOR(S):	He, Hai Yin; Faulkner, D. John
CORPORATE SOURCE:	Scripps Inst. Oceanogr., Univ. California, La Jolla, CA, 92093, USA
SOURCE:	Journal of Organic Chemistry (1989), 54(24), 5822-4 CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE:	Journal
LANGUAGE:	English
GI	



I

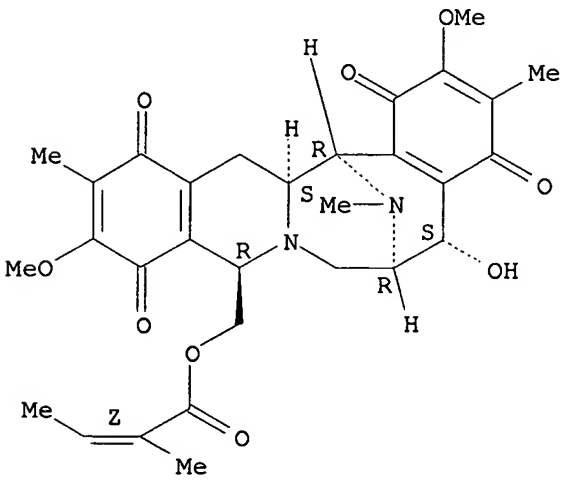
AB Renieramycins E (I, R = H) and F (I, R = MeO) are two very unstable alkaloids from the sponge Reniera sp. collected in Palau. The structure and stereochem. of renieramycins E and F were established by interpretation of spectral data. The stereochem. of renieramycin E is the same as that of the saframycins and there is good evidence to support reassignment of the stereochem. of all renieramycins. The facile decomposition of renieramycins E and F is discussed.

IT **79664-60-1 79664-61-2 79664-62-3 79664-63-4**
RL: PRP (Properties)
(configuration of)

RN 79664-60-1 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(5S,6R,9R,14aS,15R)-1,5,6,7,9,10,13,14,14a,15-decahydro-5-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

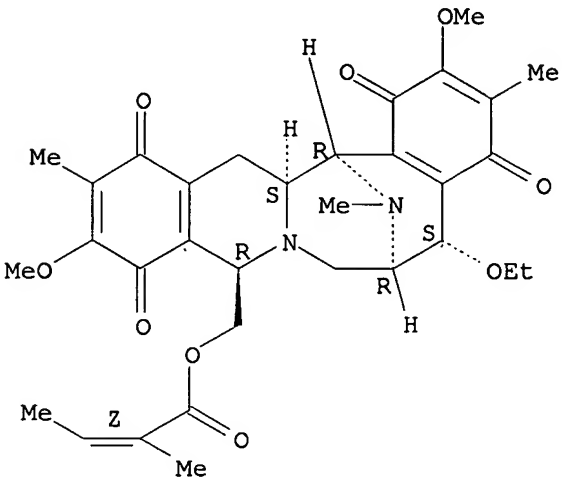


RN 79664-61-2 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(5S,6R,9R,14aS,15R)-5-ethoxy-

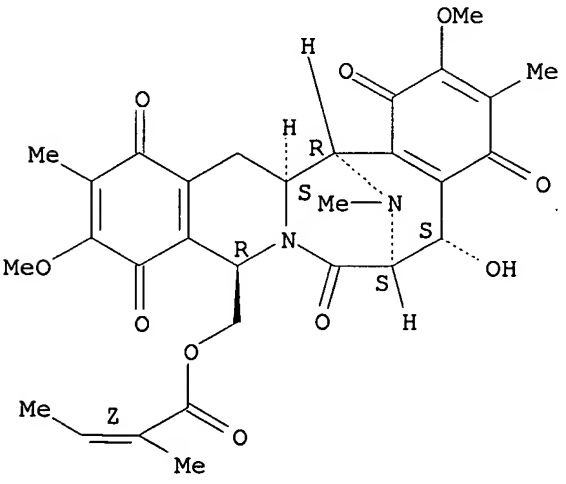
1,5,6,7,9,10,13,14,14a,15-decahydro-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



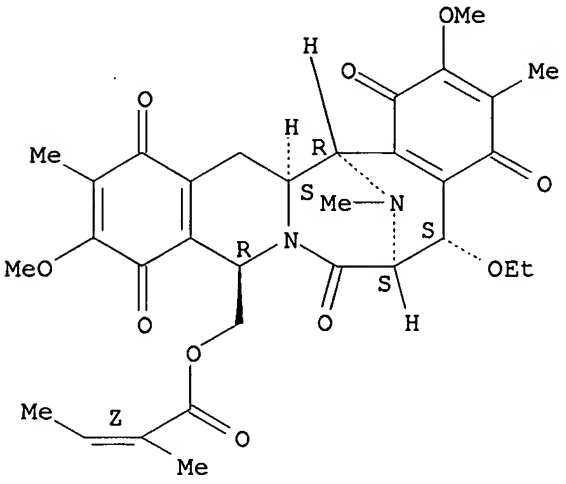
RN 79664-62-3 CAPLUS
CN 2-Butenoic acid, 2-methyl-, [(5S,6S,9R,14aS,15R)-1,5,6,7,9,10,13,14,14a,15-decahydro-5-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-1,4,7,10,13-pentaoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



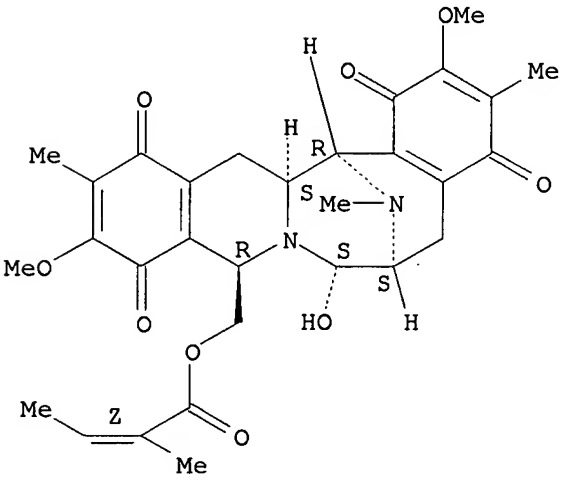
RN 79664-63-4 CAPLUS
CN 2-Butenoic acid, 2-methyl-, [(5S,6S,9R,14aS,15R)-5-ethoxy-1,5,6,7,9,10,13,14,14a,15-decahydro-2,11-dimethoxy-3,12,16-trimethyl-1,4,7,10,13-pentaoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



IT **123641-95-2 123641-96-3**
RL: BIOL (Biological study)
(isolation, mol. structure, and configuration of)
RN 123641-95-2 CAPLUS
CN 2-Butenoic acid, 2-methyl-, [(6S,7S,9R,14aS,15R)-1,5,6,7,9,10,13,14,14a,15-decahydro-7-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

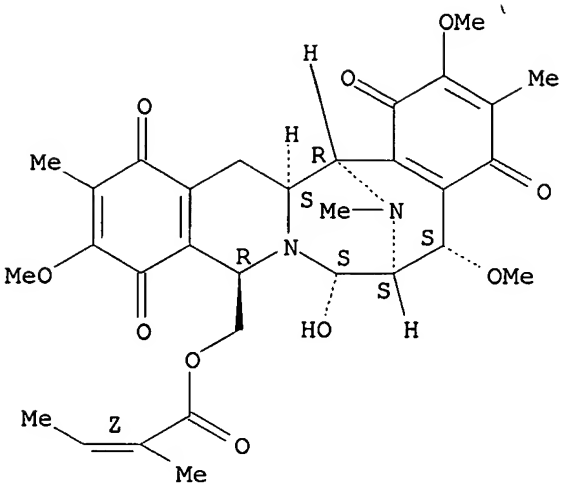
Absolute stereochemistry.
Double bond geometry as shown.



RN 123641-96-3 CAPLUS
CN 2-Butenoic acid, 2-methyl-, [(5S,6S,7S,9R,14aS,15R)-1,5,6,7,9,10,13,14,14a,15-decahydro-7-hydroxy-2,5,11-trimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

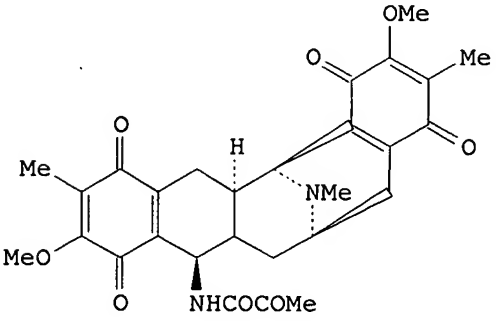
Double bond geometry as shown.



L7 ANSWER 22 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

M19

ACCESSION NUMBER: 1988:510118 CAPLUS
DOCUMENT NUMBER: 109:110118
TITLE: Stereoselective total synthesis of (±)-saframycin B
AUTHOR(S): Kubo, Akinori; Saito, Naoki; Yamato, Hidekazu; Masubuchi, Kazunao; Nakamura, Madoka
CORPORATE SOURCE: Meiji Coll. Pharm., Tokyo, 154, Japan
SOURCE: Journal of Organic Chemistry (1988), 53(18), 4295-310
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 109:110118
GI



I

AB A 20-step total synthesis of (±)-saframycin B (I) from (Z)-1-acetyl-3-arylidene-6-(arylmethyl)-2,5-piperazinedione is described.

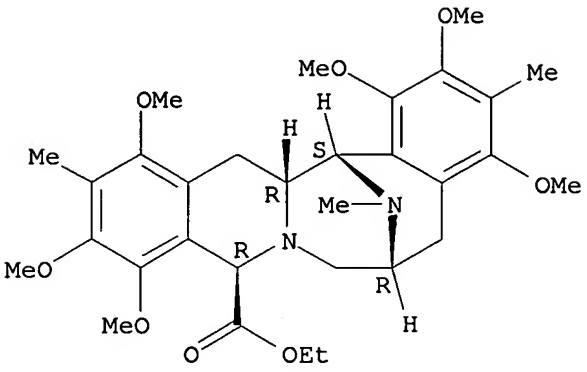
IT **112446-10-3P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)

RN 112446-10-3 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, ethyl ester, (6α,9α,14aα,15α)- (9CI) (CA INDEX

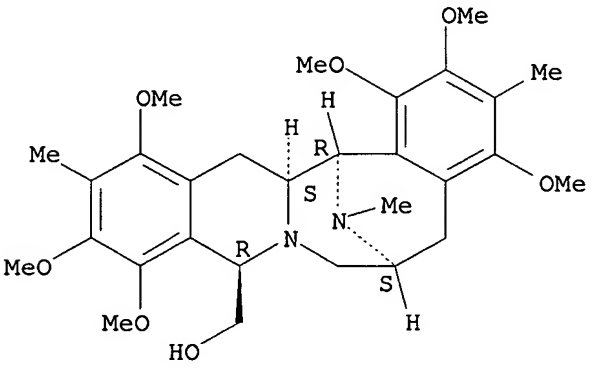
NAME)

Relative stereochemistry.



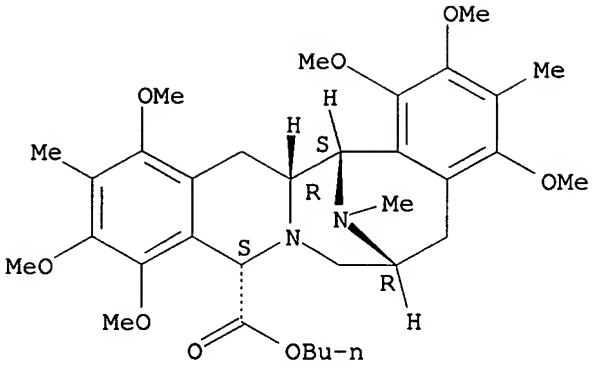
IT **112446-04-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with phthalimide)
RN 112446-04-5 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6α,9β,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



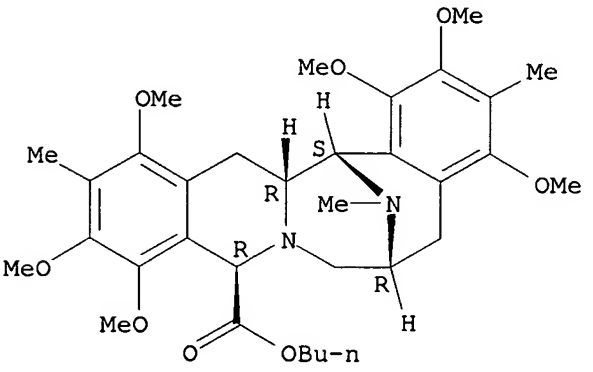
IT **112446-05-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 112446-05-6 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, butyl ester, (6α,9β,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT **112529-58-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and transesterification of)
RN 112529-58-5 CAPLUS
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, butyl ester, (6α,9α,14aα,15α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L7 ANSWER 23 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1988:473253 CAPLUS
DOCUMENT NUMBER: 109:73253
TITLE: Preparation of 6,15-iminoisoquino[3,2-b][3]benzazocine derivatives as intermediates for an antitumor agent saframycin B
INVENTOR(S): Kubo, Yotoku; Saito, Naoki
PATENT ASSIGNEE(S): Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

JP 63002991 A2 19880107 JP 1986-144916 19860623
PRIORITY APPLN. INFO.: JP 1986-144916 19860623
OTHER SOURCE(S): MARPAT 109:73253
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

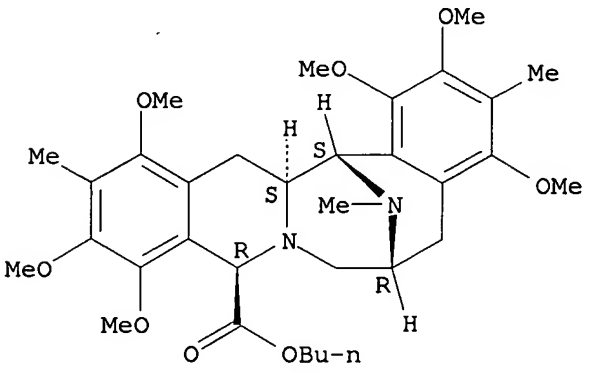
AB Isoquinolines I (R = CH2OH, CH2NH2, phthaloylmethyl) (II) are prepared from diazabicyclononane III. A mixture of III and K2CO3 in BuOH was treated with OHCCO2Bu at room temperature for 67 h and the concentrated reaction mixture was stirred in CF3CO2H at ice-cooled temperature for 1 h to give 70.2% isoquinoline IV, which was isomerized by treatment with Hg(OAc)2 in AcOH and then H2S(g), followed by NaBH4 treatment of the product in EtOH in the presence of NaHCO3 to give 70.6% I (R = CO2Bu) (V). A mixture of V and LiAlH4 in THF was refluxed for 2 h to afford 76.8% I (R = CH2OH), which was converted to saframycin B in 4 steps.

IT **115510-17-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and LAH reduction of, in preparation of saframycin B)

RN 115510-17-3 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, butyl ester, [6R-(6α,9α,14aβ,15α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **115510-16-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and isomerization of, in preparation of saframycin B)

RN 115510-16-2 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, butyl ester, [6R-(6α,9β,14aβ,15α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.